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=> d his ful

     (FILE 'HOME' ENTERED AT 10:16:30 ON 14 OCT 2005)

     FILE 'HCAPLUS' ENTERED AT 10:16:34 ON 14 OCT 2005
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                E WO99-GB03295/APPS
                E WO99-GB3295/APPS
L1            1 SEA ABB=ON  PLU=ON  (WO99-GB3295/AP OR WO99-GB3295/PRN)
                D SCA TI
                SEL RN

     FILE 'REGISTRY' ENTERED AT 10:18:53 ON 14 OCT 2005
L2          156 SEA ABB=ON  PLU=ON  (101421-76-5/BI OR 104-97-2/BI OR 109-01-3/
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                 OR 121-34-6/BI OR 123855-51-6/BI OR 13790-39-1/BI OR 13794-72-
                4/BI OR 142851-03-4/BI OR 1479-24-9/BI OR 1572-10-7/BI OR
                1578-89-8/BI OR 1615-14-1/BI OR 16499-57-3/BI OR 166815-96-9/BI
                 OR 179688-01-8/BI OR 18997-19-8/BI OR 193002-24-3/BI OR
                193002-25-4/BI OR 193002-30-1/BI OR 193002-31-2/BI OR 193002-32
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                199328-78-4/BI OR 2033-24-1/BI OR 2058-49-3/BI OR 208519-10-2/B
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L3           83 SEA ABB=ON  PLU=ON  L2 AND NCNC3/ESS
L4       376959 SEA ABB=ON  PLU=ON  NCNC3/ESS(S)C6/ESS
L5           83 SEA ABB=ON  PLU=ON  L2 AND L4

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L6            1 SEA ABB=ON  PLU=ON  L1 AND L5
                D L6 IALL HITSTR

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L8            8 SEA SSS SAM L7
L9          138 SEA SSS FUL L7
L10          38 SEA ABB=ON  PLU=ON  L9 AND L2

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L11           1 SEA ABB=ON  PLU=ON  L10
L12           1 SEA ABB=ON  PLU=ON  L1 AND L11
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L13          29 SEA ABB=ON  PLU=ON  L9
L14           9 SEA ABB=ON  PLU=ON  L13 NOT PY>1998
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L15          27 SEA SSS FUL L7
L16           4 SEA ABB=ON  PLU=ON  L9
L17          23 SEA ABB=ON  PLU=ON  L15 NOT L16


     FILE HOME

     FILE HCAPLUS

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     FILE COVERS 1907 - 14 Oct 2005  VOL 143 ISS 17
     FILE LAST UPDATED: 13 Oct 2005  (20051013/ED)

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      This file contains CAS Registry Numbers for easy and accurate
      substance identification.

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   12 OCT 2005  HIGHEST RN 865114-63-2
     DICTIONARY FILE UPDATES:  12 OCT 2005  HIGHEST RN 865114-63-2

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.

     ************************************************************
     *                                                          *
     * The CA roles and document type information have been removed from *
     * the IDE default display format and the ED field has been added,   *
     * effective March 20, 2005.  A new display format, IDERL, is now    *
     * available and contains the CA role and document type information. *
     *                                                          *
     ************************************************************

     Structure search iteration limits have been increased.  See HELP SLIMITS
     for details.

     REGISTRY includes numerically searchable data for experimental and
```

predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE BEILSTEIN
FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.
FILE CONTAINS 9,363,954 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW

*** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**

*** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**

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=> d que stat l13
L7                STR
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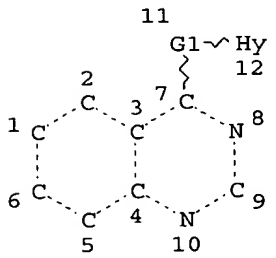


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CONNECT IS E2  RC AT   9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
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ECOUNT IS M2-X5 C AT 12

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L9 138 SEA FILE=REGISTRY SSS FUL L7
L13 29 SEA FILE=HCAPLUS ABB=ON PLU=ON L9

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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L13 ANSWER 1 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:962244 HCAPLUS
DOCUMENT NUMBER: 143:266946
TITLE: Preparation of pyridines and related compounds as TGF-β inhibitors
INVENTOR(S): Shimizu, Kiyoshi; Shimizu, Toshiyuki; Kawakami, Kazuki; Nakoji, Masayoshi; Sakai, Teruyuki
PATENT ASSIGNEE(S): Kirin Beer Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 461 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080377	A1	20050901	WO 2005-JP2610	20050218

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2004-45383 A 20040220
GI

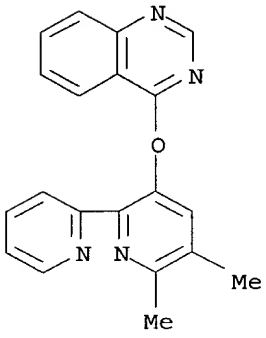
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = II; Z = O, etc.; D1, D2, D3, D4, X, E, G, J, L, M = C, N; further details on D1, D2, D3, D4, X, E, G, J, L, M are given.; R1-R6, R10-R14 = H, halo, etc.] were prepared For example, reaction of 4-chloro-6,7-dimethoxyquinazoline with 5,6-dimethyl-[2,2'-bipyridin]-3-ol, e.g., prepared from 2,3-dimethylfuran in 2 steps, afforded compound III in 81% yield. In TGF-β signal inhibition assays (in vitro), compound III

exhibited the inhibitory activity of 89% at 1 μM. Compds. I are claimed useful for the treatment of arthritis, ulcer, etc.

IT **863783-82-8P 863783-83-9P 863783-84-0P 863783-85-1P 863783-86-2P 863783-96-4P 863783-97-5P 863783-98-6P 863784-03-6P 863786-57-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridines and related compds. as TGF-β inhibitors for treatment of arthritis, ulcer, etc.)

RN 863783-82-8 HCAPLUS
CN Quinazoline, 4-[(5,6-dimethyl[2,2'-bipyridin]-3-yl)oxy]- (9CI) (CA INDEX NAME)



RN 863783-83-9 HCAPLUS
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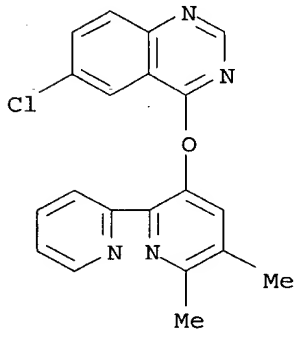

RN 863783-84-0 HCAPLUS
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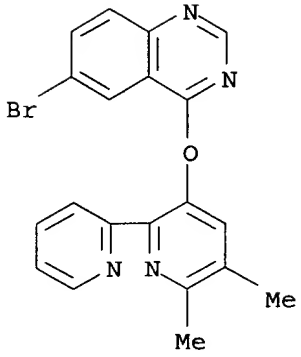

RN 863783-85-1 HCAPLUS
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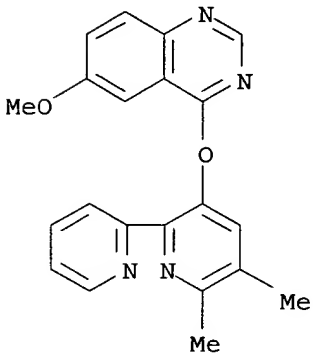
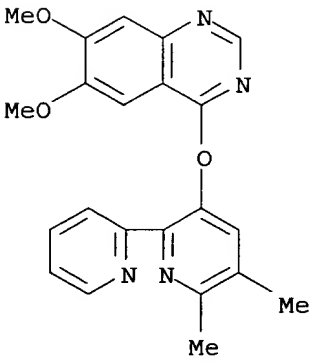
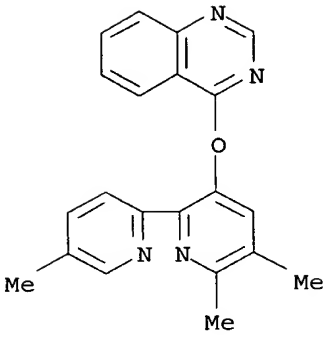


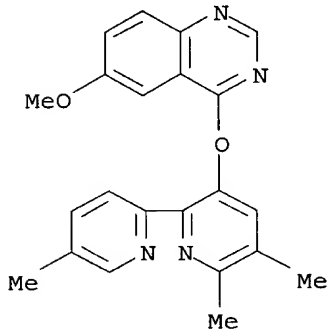
RN 863783-86-2 HCAPLUS
CN Quinazoline, 4-[(5,6-dimethyl[2,2'-bipyridin]-3-yl)oxy]-6,7-dimethoxy- (9CI) (CA INDEX NAME)



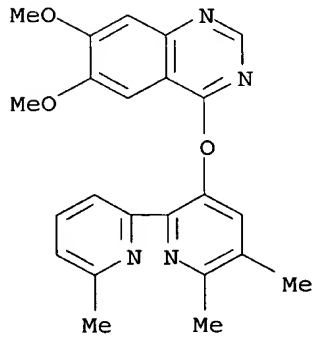
RN 863783-96-4 HCAPLUS
CN Quinazoline, 4-[(5,5',6-trimethyl[2,2'-bipyridin]-3-yl)oxy]- (9CI) (CA INDEX NAME)



RN 863783-97-5 HCAPLUS
CN Quinazoline, 6-methoxy-4-[(5,5',6-trimethyl[2,2'-bipyridin]-3-yl)oxy]-
(9CI) (CA INDEX NAME)



RN 863783-98-6 HCAPLUS
CN Quinazoline, 6,7-dimethoxy-4-[(5,6,6'-trimethyl[2,2'-bipyridin]-3-yl)oxy]-
(9CI) (CA INDEX NAME)



RN 863784-03-6 HCAPLUS
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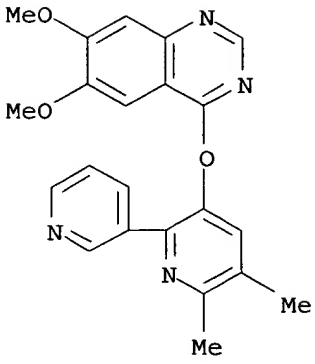
(9CI) (CA INDEX NAME)



RN 863786-57-6 HCAPLUS
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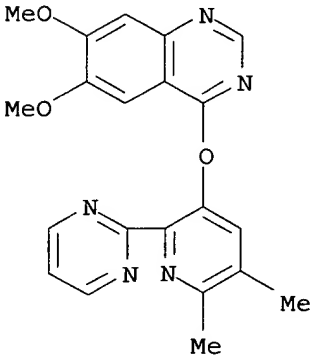
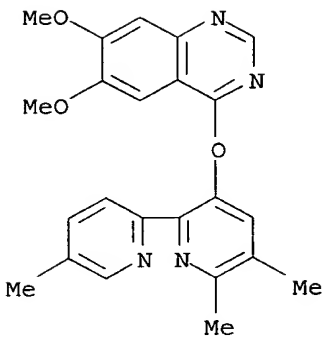


IT **666734-04-9**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of pyridines and related compds. as TGF-β inhibitors for treatment of arthritis, ulcer, etc.)
RN 666734-04-9 HCAPLUS
CN Quinazoline, 6,7-dimethoxy-4-[(5,5',6-trimethyl[2,2'-bipyridin]-3-yl)oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:735319 HCAPLUS
DOCUMENT NUMBER: 143:211837
TITLE: Preparation of tetrahydropyranones as hepatitis C virus RNA-dependent RNA polymerase inhibitors
INVENTOR(S): Borchardt, Allen; Gonzalez, Javier; Li, Hui; Linton, Maria Angelica; Tatlock, John Howard
PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 251 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005176701	A1	20050811	US 2003-718337	20031119
PRIORITY APPLN. INFO.:			US 2003-718337	20031119

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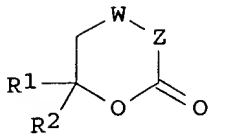

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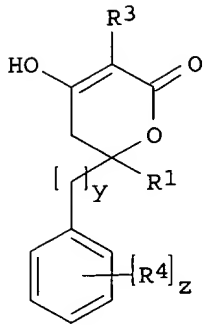

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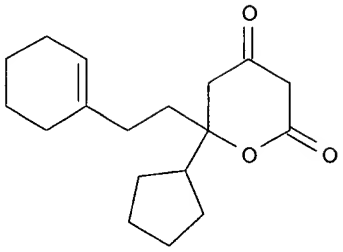


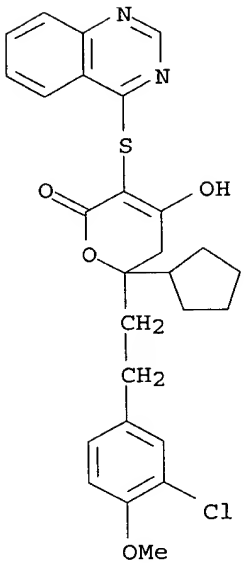
III

AB Title compds. I [wherein WZ = COCHR3, C(OR6)=CR3'; R1 = independently H, (un)substituted (cyclo)alkyl, alkenyl, alkynyl, heterocyclyl, or aryl; R2 = R1, (un)substituted arylalkyl, heterocyclylalkyl, arylalkoxy, or heterocyclylalkoxy, etc.; R3 = H, OR6, SR6, NR6R7, R2; R3' = R3 except H; R6, R7 = independently H, (un)substituted (cyclo)alkyl, aryl(alkyl), or heterocyclyl(alkyl); and pharmaceutically acceptable salts, solvates, prodrugs, and metabolites thereof] such as II [R1 = cyclopentyl; R3 = (CR8R9)t[(un)substituted 4-10 membered heterocyclyl] (wherein t = 0-5; R8, R9 = H); R4 = halo, alkyl, hydroxy, alkoxy, etc.; z = 1-5; y = 0-5], including purine derivs., were prepared as hepatitis C virus (HCV) RNA-dependent RNA polymerase (RdRp) inhibitors. For example, 3-(cyclohex-1-enyl)propionic acid Et ester was hydrolyzed with LiOH in THF/MeOH to give the acid, which was esterified with 2,2'-dipyridyl disulfide in CH2CH2 to provide 3-(cyclohex-1-enyl)thiopropionic acid S-(pyridin-2-yl) ester (93%). Reaction of the thioester with cyclopentylmagnesium bromide in THF afforded 3-(cyclohex-1-enyl)-1-cyclopentylpropan-1-one (72%). Coupling of the ketone with Me acetoacetate in the presence of NaH and BuLi in THF produced the 2,4-pyrandione III (40%). Compds. of the invention inhibited the ability of recombinant HCV polymerase to perform primer/template-directed transcription in vitro with IC50 values ranging from 0.001 μM to 83 μM. Thus, I and pharmaceutical compns. are useful for treating Hepatitis C virus in mammals (no data).

IT **749933-73-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(HCV polymerase inhibitor; preparation of pyranones as HCV polymerase inhibitors)

RN 749933-73-1 HCAPLUS

CN 2H-Pyran-2-one, 6-[2-(3-chloro-4-methoxyphenyl)ethyl]-6-cyclopentyl-5,6-dihydro-4-hydroxy-3-(4-quinazolinylthio)- (9CI) (CA INDEX NAME)



L13 ANSWER 3 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:490266 HCAPLUS
DOCUMENT NUMBER: 143:40007
TITLE: AKT protein kinase inhibitors for use in treatment of hyperproliferative diseases
INVENTOR(S): Mitchell, Ian S.; Spencer, Keith L.; Stengel, Peter; Han, Yongxin; Kallan, Nicholas C.; Munson, Mark; Vigers, Guy P. A.; Blake, James; Piscopio, Anthony; Josey, John; Miller, Scott; Xiao, Dengming; Xu, Riu; Rao, Chang; Wang, Bin; Bernacki, April L.
PATENT ASSIGNEE(S): Array Biopharma Inc., USA
SOURCE: PCT Int. Appl., 234 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

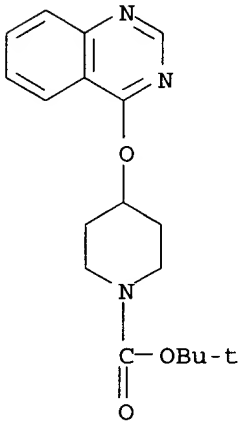
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051304	A2	20050609	WO 2004-US39094	20041119
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005130954	A1	20050616	US 2004-993173	20041119

PRIORITY APPLN. INFO.: US 2003-524003P P 20031121
OTHER SOURCE(S): MARPAT 143:40007

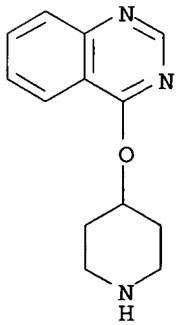
AB The present invention provides compds., including resolved enantiomers, diastereomers, solvates and pharmaceutically acceptable salts thereof, and methods of using the compds. of this invention as AKT protein kinase inhibitors and for the treatment of hyperproliferative diseases such as cancer. Thus, over 100 compds. were synthesized. Several of these compds., including (2R)-2-amino-3-(4-chlorophenyl)-1-(4-quinazolin-4-ylpiperazin-1-yl)propan-1-one, (2R)-2-amino-3-(2-naphthyl)-1-(4-quinazolin-4-ylpiperazin-1-yl)propan-1-one, and (2R)-2-amino-3-(4-chlorophenyl)-1-(4-thieno[3,2,b]pyridin-7-yl-piperazin-1-yl)propan-1-one inhibited human AKT-1 protein kinase in in vitro assays.

IT **853680-41-8P 853680-42-9P 853680-43-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(AKT protein kinase inhibitors for use in treatment of hyperproliferative diseases)

RN 853680-41-8 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinyloxy)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 853680-42-9 HCAPLUS
CN Quinazoline, 4-(4-piperidinyloxy)-, dihydrochloride (9CI) (CA INDEX NAME)

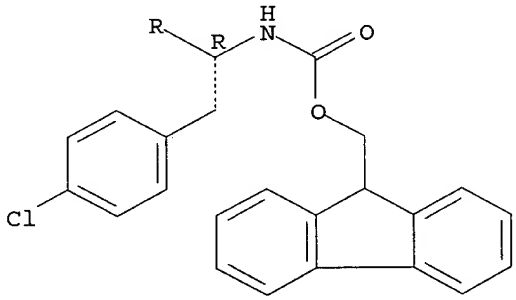


●2 HCl

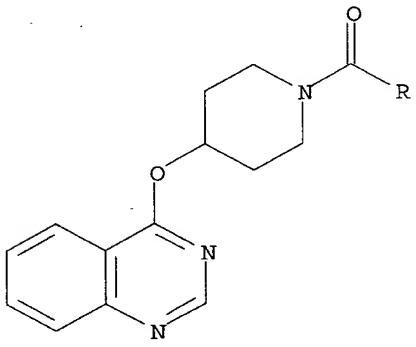
RN 853680-43-0 HCAPLUS
CN Carbamic acid, [(1R)-1-[(4-chlorophenyl)methyl]-2-oxo-2-[4-(4-quinazolinyloxy)-1-piperidinyl]ethyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

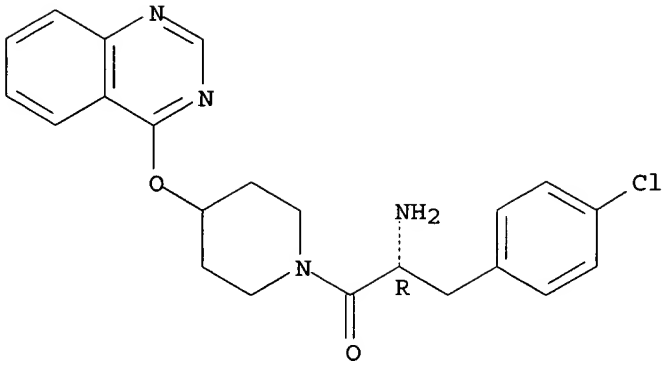


PAGE 2-A



IT **853679-07-9P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(AKT protein kinase inhibitors for use in treatment of hyperproliferative diseases)
RN 853679-07-9 HCAPLUS
CN Piperidine, 1-[(2R)-2-amino-3-(4-chlorophenyl)-1-oxopropyl]-4-(4-quinazolinyloxy)-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

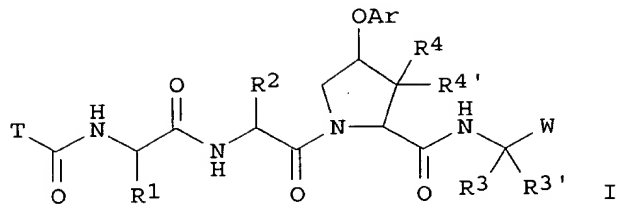


●2 HCl

L13 ANSWER 4 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:347009 HCAPLUS
DOCUMENT NUMBER: 142:411657
TITLE: Preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease
INVENTOR(S): Perni, Robert B.; Court, John J.; Britt, Shawn D.; Pitlik, Janos; Van Drie, John H.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005035525	A2	20050421	WO 2004-US29093	20040907
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005137139	A1	20050623	US 2004-936450	20040907
PRIORITY APPLN. INFO.:			US 2003-500670P P	20030905

OTHER SOURCE(S): MARPAT 142:411657
GI



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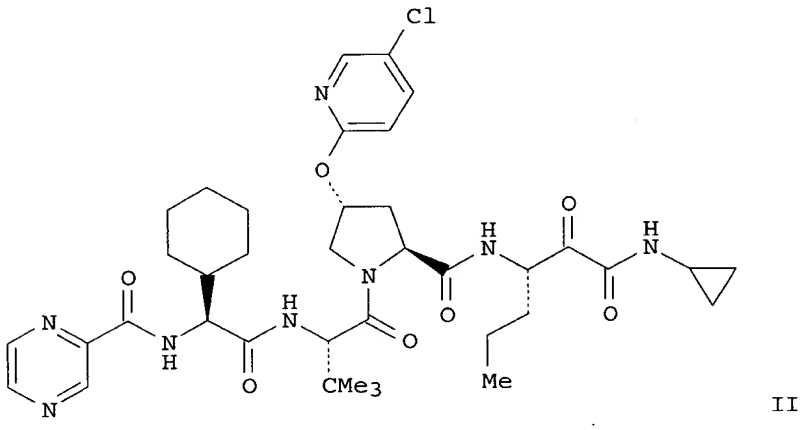


II

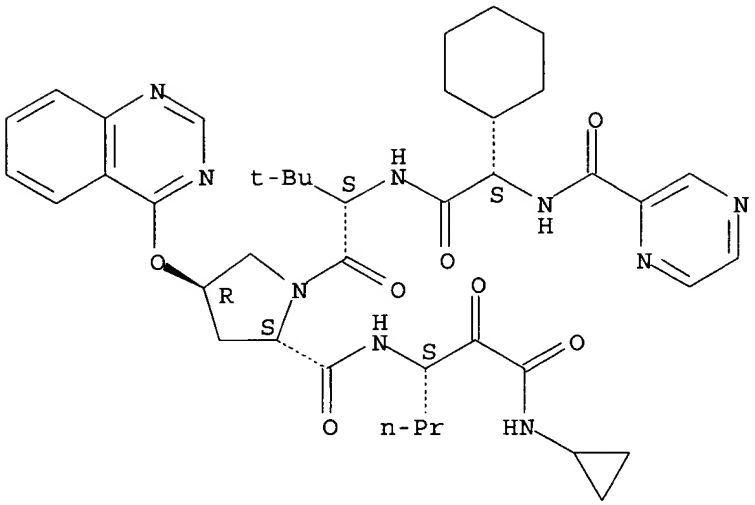
AB The invention relates to compds. I [Ar is a 5- to 10-membered aromatic ring having up to 4 heteroatoms O, S, NH, SO and SO2, in which 1-3 ring atoms are optionally substituted; R1, R2 are independently (un)substituted (hetero)alkyl, cycloalk(en)yl, cycloalk(en)yl-, aryl- or heteroaryl-(hetero)alkyl; R3, R3' are independently H, (un)substituted alkyl, halo-, sulfhydryl- or hydroxyalkyl, Ph or benzyl; or R3R3' is a ring; R4, R4' are independently H, (un)substituted (hetero)alkyl, cycloalkyl(hetero)alkyl, aryl or heterocyclyl; W is COCOR6, COCO2R6, COCONR62 (R6 is H, alkyl, (hetero)aryl, etc.) or a boryl group; T is alkyl, (hetero)aryl or (hetero)alkyl] that inhibit serine protease activity, particularly the activity of hepatitis C virus (HCV) NS3-NS4A protease. The invention further relates to processes for preparing these compds. and to pharmaceutical compns. containing them. Thus, peptide II was prepared via peptide coupling reactions in solution and shown to have HCV NS3-NS4A protease inhibitory activity (Ki < 0.1 μM and IC50 < 0.5 μM).

IT **850251-16-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease)

RN 850251-16-0 HCAPLUS

CN L-Prolinamide, (2S)-2-cyclohexyl-N-(pyrazinylcarbonyl)glycyl-3-methyl-L-valyl-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-4-(4-quinazolinyloxy)-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

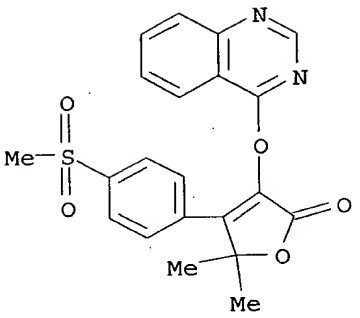


L13 ANSWER 5 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:815644 HCAPLUS
DOCUMENT NUMBER: 141:420034
TITLE: Quantitative structure activity relationship studies of diaryl furanones as selective COX-2 inhibitors
AUTHOR(S): Shahapurkar, S.; Pandya, T.; Kawathekar, N.; Chaturvedi, S. C.
CORPORATE SOURCE: Devi Ahilya Vishwavidyalaya, Takshashila Parisar, School of Pharmacy, Indore, India
SOURCE: European Journal of Medicinal Chemistry (2004), 39(10), 899-904
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Selective COX-2 inhibitors have attracted much attention in recent times in the design of non-steroidal anti-inflammatory agents (NSAID), which are devoid of the common side effects of classical NSAIDs. QSAR studies have been performed on a series of diaryl furanones that acts as selective COX-2 inhibitor using Mol. Operating Environment (MOE). The studies were carried out on 43 analogs. These studies produced good predictive models and give statistically significant correlations of selective COX-2 inhibitory with phys. property, connectivity and conformation of mol. Also when available COX-1 inhibitory data was analyzed with descriptors obtained from MOE, partial charge descriptor, van der Waal's surface area and solvation energy gave statistically significant results.

IT **189955-00-8**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR studies of diaryl furanones as selective COX-2 inhibitors)

RN 189955-00-8 HCAPLUS
CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

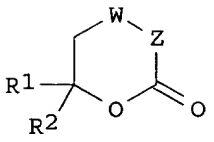
L13 ANSWER 6 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:718528 HCAPLUS
DOCUMENT NUMBER: 141:243338
TITLE: Preparation of tetrahydropyranones as hepatitis C virus RNA-dependent RNA polymerase inhibitors
INVENTOR(S): Borchardt, Allen John; Gonzalez, Javier; Li, Hui; Linton, Maria Angelica; Tatlock, John Howard
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: PCT Int. Appl., 527 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004074270	A2	20040902	WO 2004-IB493	20040209
WO 2004074270	A3	20041223		
WO 2004074270	B1	20050317		
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004224960	A1	20041111	US 2004-783117	20040217
NL 1025544	A1	20040824	NL 2004-1025544	20040220

PRIORITY APPLN. INFO.:

US 2003-449088P	P	20030221
US 2003-472355P	P	20030520

OTHER SOURCE(S): MARPAT 141:243338
GI



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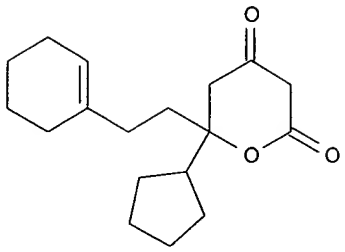


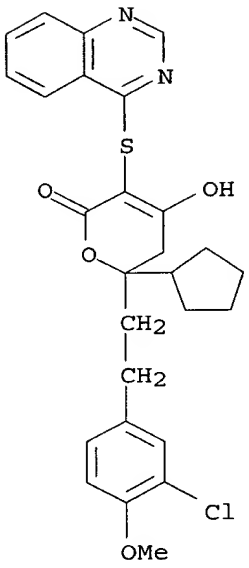
II

AB Title compds. I [wherein WZ = COCHR3, C(OR6)=CR3'; R1 = independently H, (un)substituted (cyclo)alkyl, alkenyl, alkynyl, heterocyclyl, or aryl; R2 = R1, (un)substituted arylalkyl, heterocyclylalkyl, arylalkoxy, or heterocyclylalkoxy, etc.; R3 = H, OR6, SR6, NR6R7, R2; R3' = R3 except H; R6, R7 = independently H, (un)substituted (cyclo)alkyl, aryl(alkyl), or heterocyclyl(alkyl); and pharmaceutically acceptable salts, solvates, prodrugs, and metabolites thereof], including purine derivs., were prepared as hepatitis C virus (HCV) RNA-dependent RNA polymerase (RdRp) inhibitors. For example, 3-(cyclohex-1-enyl)propionic acid Et ester was hydrolyzed with LiOH in THF/MeOH to give the acid, which was esterified with 2,2'-dipyridyl disulfide in CH2CH2 to provide 3-(cyclohex-1-enyl)thiopropionic acid S-(pyridin-2-yl) ester (93%). Reaction of the thioester with cyclopentylmagnesium bromide in THF afforded 3-(cyclohex-1-enyl)-1-cyclopentylpropan-1-one (72%). Coupling of the ketone with Me acetoacetate in the presence of NaH and BuLi in THF produced the 2,4-pyrandione II (40%). Compds. of the invention inhibited the ability of recombinant HCV polymerase to perform primer/template-directed transcription in vitro with IC50 values ranging from 0.001 μM to 83 μM. Thus, I and pharmaceutical compns. are useful for treating Hepatitis C virus in mammals (no data).

IT **749933-73-1P**, 6-[2-(3-Chloro-4-methoxyphenyl)ethyl]-6-cyclopentyl-4-hydroxy-3-[(quinazolin-4-yl)thio]-5,6-dihydro-2H-pyran-2-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(HCV polymerase inhibitor; preparation of pyranones as HCV polymerase inhibitors)

RN 749933-73-1 HCAPLUS

CN 2H-Pyran-2-one, 6-[2-(3-chloro-4-methoxyphenyl)ethyl]-6-cyclopentyl-5,6-dihydro-4-hydroxy-3-(4-quinazolinylthio)- (9CI) (CA INDEX NAME)

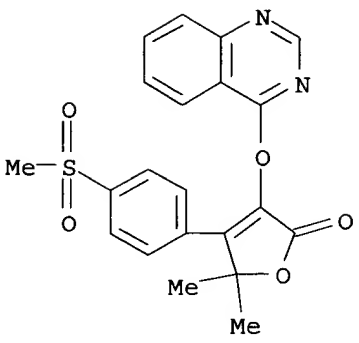


L13 ANSWER 7 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:303493 HCAPLUS
DOCUMENT NUMBER: 141:16893
TITLE: Quantitative structure activity relationship studies of diaryl furanones as selective COX-2 inhibitors
AUTHOR(S): Shahapurkar, S.; Pandya, T.; Kawathekar, N.; Chaturvedi, S. C.
CORPORATE SOURCE: School of Pharmacy, Indore, India
SOURCE: European Journal of Medicinal Chemistry (2004), 39(4), 383-388
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Selective COX-2 inhibitors have attracted much attention in recent times in the design of non-steroidal anti-inflammatory agents (NSAID), which are devoid of the common side effects of classical NSAIDs. QSAR studies have been performed on a series of diaryl furanones that acts as selective COX-2 inhibitor using Mol. Operating Environment (MOE). The studies were carried out on 43 analogs. These studies produced good predictive models and give statistically significant correlations of selective COX-2 inhibitory with phys. property, connectivity and conformation of mol. Also when available COX-1 inhibitory data was analyzed with descriptors obtained from MOE, partial charge descriptor, van der Waal's surface area and solvation energy gave statistically significant results.

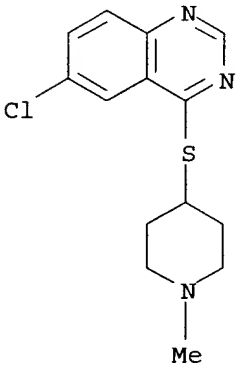
IT **189955-00-8**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(quant. structure activity relationship studies of diaryl furanones as selective COX-2 inhibitors)

RN 189955-00-8 HCAPLUS
CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:205966 HCAPLUS
DOCUMENT NUMBER: 142:197901
TITLE: Product class 13: quinazolines
AUTHOR(S): Kikelj, D.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2004), 16, 573-749
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Preparation of quinazolines by ring closure and ring transformation reactions as well as aromatization and substituent modification is given.
IT **325145-98-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of quinazolines)
RN 325145-98-0 HCAPLUS
CN Quinazoline, 6-chloro-4-[(1-methyl-4-piperidinyl)thio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1014 THERE ARE 1014 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

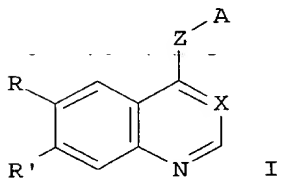
L13 ANSWER 9 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:182845 HCAPLUS

DOCUMENT NUMBER: 140:217519
TITLE: Preparation of quinoline derivatives as TGFβ inhibitors
INVENTOR(S): Shimizu, Kiyoshi; Shimizu, Toshiyuki; Kimura, Kaname; Kawakami, Kazuki; Nakoji, Masayoshi
PATENT ASSIGNEE(S): Kirin Beer Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 628 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018430	A1	20040304	WO 2003-JP10647	20030822
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1548008	A1	20050629	EP 2003-792805	20030822
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: JP 2002-244028 A 20020823
WO 2003-JP10647 W 20030822

OTHER SOURCE(S): MARPAT 140:217519
GI

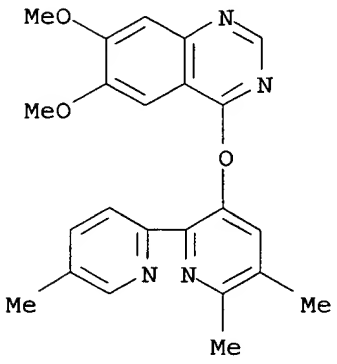


I

AB The title compds. I [wherein X = CH or N; Z = O, NH, S, or CO; R and R' = independently H, halo, (un)substituted alkyl, alkenyl, NH2, CONH2, OH, or heterocyclyl; A = (un)substituted Ph or (hetero)cyclyl] or pharmaceutically acceptable salts, or solvates thereof are prepared as transforming growth factor (TGF) β inhibitors. For example, 4-chloro-6,7-dimethoxyquinoline was reacted with 2-benzylphenol in 1,2-dichlorobenzene to give 4-(2-benzylphenoxy)-6,7-dimethoxyquinoline (10%). Some of compds. I inhibited 100% of human TGFβ at 10 μM.

IT **666734-04-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of quinoline derivs. as TGFβ inhibitors)
RN 666734-04-9 HCAPLUS
CN Quinazoline, 6,7-dimethoxy-4-[(5,5',6-trimethyl[2,2'-bipyridin]-3-yl)oxy]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 10 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:162461 HCAPLUS
DOCUMENT NUMBER: 140:217653
TITLE: Preparation of heterocyclic-substituted quinolines/quinazolines and related compounds as Inhibitors of JAK protein kinase
INVENTOR(S): Bemis, Guy W.; Harbeson, Scott L.; Ledeboer, Mark
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 58 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004038992	A1	20040226	US 2003-430805	20030506
CA 2485429	AA	20040715	CA 2003-2485429	20030506
WO 2004058753	A1	20040715	WO 2003-US14223	20030506
WO 2004058753	C1	20050616		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1501829	A1	20050202	EP 2003-799762	20030506
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: US 2002-378185P P 20020506

WO 2003-US14223 A 20030506

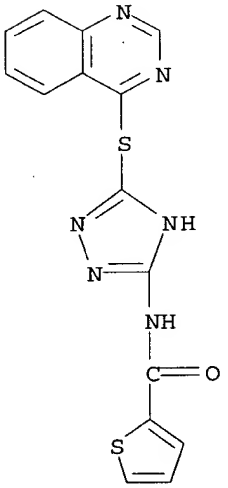
OTHER SOURCE(S): MARPAT 140:217653
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

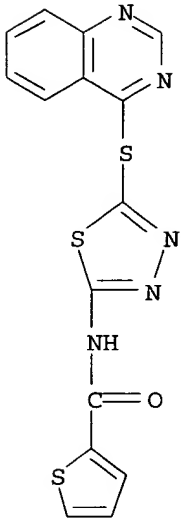
AB Title compds. I [W, X = O, S; A = N, CH, CCN, C-alkyl; R1-2 = taken together form an (un)substituted 3-7 membered (un)saturated (hetero)cycle; Q = bond, CO, carboxamido, etc.; R3 = alkyl, (un)substituted 3-8 membered monocyclic or 8-10 membered bicyclic ring, etc.] are prepared For instance, 5-((7-chloroquinolin-4-yl)oxy)-1,3,4-thiadiazole-2-carboxylic acid N-((furan-2-yl)methyl)amide (II) is prepared from ((furan-2-yl)methyl)amine and the corresponding thiadiazole Et ester (DME, 80°, 18 h). Certain example compds. have IC50 between 2 and 5 μM for JAK kinase. I are useful in the treatment of a neurodegenerative disorder, an autoimmune disorder, etc.

IT **664324-74-7P 664324-81-6P 664325-06-8P**
664325-07-9P 664325-13-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic-substituted quinolines/quinazolines and related compds. as Inhibitors of jak protein kinase)

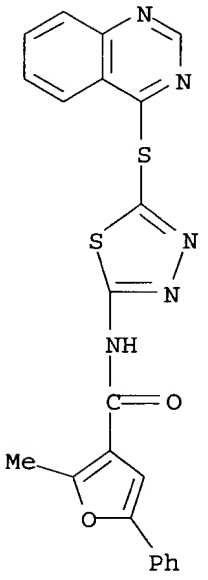
RN 664324-74-7 HCAPLUS
CN 2-Thiophenecarboxamide, N-[5-(4-quinazolinylthio)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)



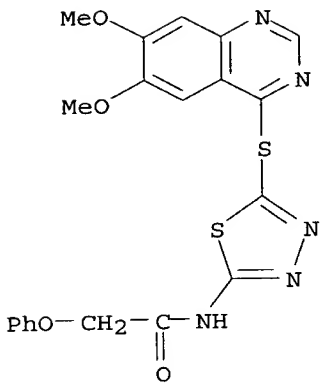
RN 664324-81-6 HCAPLUS
CN 2-Thiophenecarboxamide, N-[5-(4-quinazolinylthio)-1,3,4-thiadiazol-2-yl]- (9CI) (CA INDEX NAME)



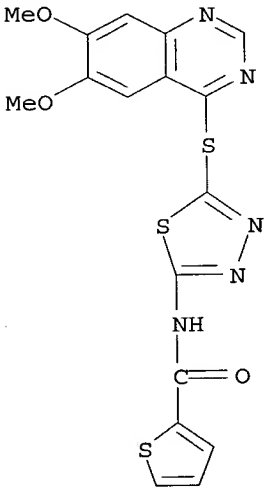
RN 664325-06-8 HCAPLUS
CN 3-Furancarboxamide, 2-methyl-5-phenyl-N-[5-(4-quinazolinylthio)-1,3,4-thiadiazol-2-yl]- (9CI) (CA INDEX NAME)



RN 664325-07-9 HCAPLUS
CN Acetamide, N-[5-[(6,7-dimethoxy-4-quinazolinyl)thio]-1,3,4-thiadiazol-2-yl]-2-phenoxy- (9CI) (CA INDEX NAME)



RN 664325-13-7 HCAPLUS
CN 2-Thiophenecarboxamide, N-[5-[(6,7-dimethoxy-4-quinazolinyl)thio]-1,3,4-thiadiazol-2-yl]- (9CI) (CA INDEX NAME)

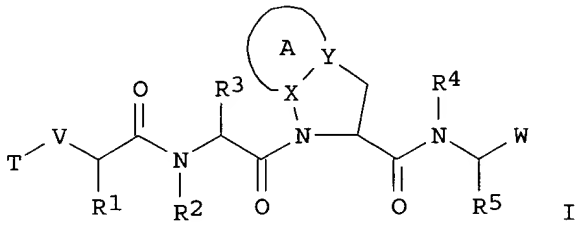


L13 ANSWER 11 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:837079 HCAPLUS
DOCUMENT NUMBER: 139:338195
TITLE: Preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease
INVENTOR(S): Pitlik, Janos; Cottrell, Kevin M.; Farmer, Luc J.; Perni, Robert B.; Courtney, Lawrence F.; Van Drie, John H.; Murcko, Mark A.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 210 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

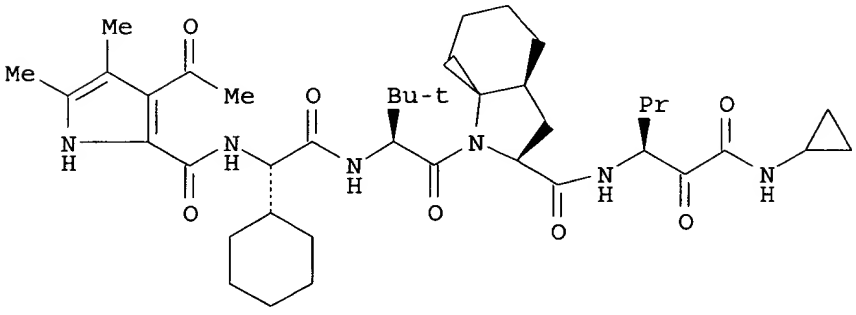
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003087092	A2	20031023	WO 2003-US11459	20030411
WO 2003087092	A3	20040910		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2481369	AA	20031023	CA 2003-2481369	20030411
EP 1497282	A2	20050119	EP 2003-719741	20030411
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			US 2002-371846P	P 20020411
			WO 2003-US11459	W 20030411

OTHER SOURCE(S): MARPAT 139:338195

GI



I



II

AB The invention relates to compds. I [A together with X and Y is a 3- to 6-membered aromatic or non-aromatic ring having up to 3 heteroatoms; R1, R3 are aliphatic, (un)substituted (cyclo)alk(en)yl, (hetero)aryl, etc.; R2, R4 are H, (un)substituted aliphatic, cycloalkyl or aryl aliphatic; R5 is (un)substituted aliphatic; W is COCOR6, COCO2R6, or COCONR62, where R6 is H, aliphatic, (hetero)aryl, etc.; V is CONR8, SONR8, SO2NR8, where R8 is H or aliphatic; T is (hetero)aryl, aliphatic, sulfonylaminoalkyl, etc.] that inhibit serine protease activity, particularly the activity of hepatitis C virus NS3-NS4A protease. Thus, peptide II was prepared via coupling reactions in

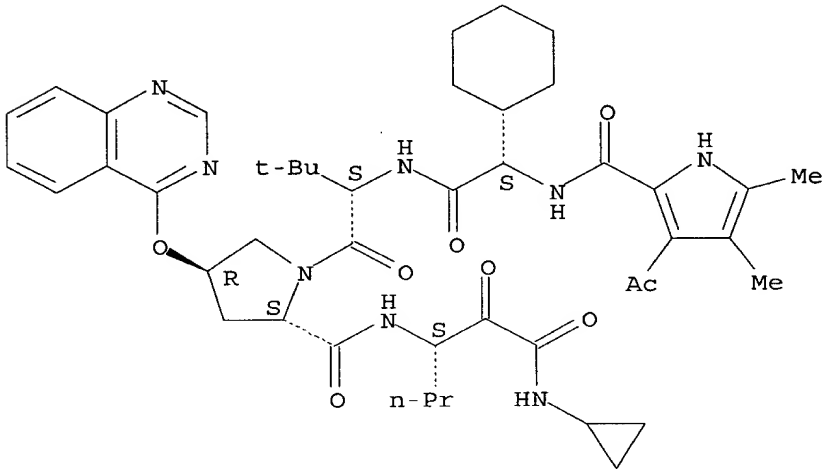
solution and showed Ki and IC50 values < 0.5 μM.

IT **615584-04-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease)

RN 615584-04-8 HCAPLUS

CN L-Prolinamide, 3-acetyl-2,3,4,5-tetradehydro-4,5-dimethylprolyl-(2S)-2-cyclohexylglycyl-3-methyl-L-valyl-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-4-(4-quinazolinyloxy)-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 12 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:276519 HCAPLUS
DOCUMENT NUMBER: 136:310188
TITLE: Treatment of cancer with a prostate specific antigen (PSA) conjugate and an NSAID compound
INVENTOR(S): Heimbrook, David C.; Yao, Siu-long
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 129 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002042375	A1	20020411	US 2001-896245		20010629
PRIORITY APPLN. INFO.:			US 2000-216217P	P	20000705

OTHER SOURCE(S): MARPAT 136:310188

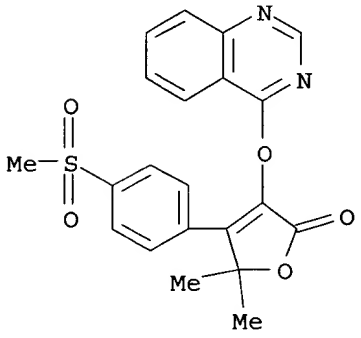
AB The invention relates to methods of treating cancer using a combination of a compound which is a PSA conjugate and a nonsteroidal antiinflammatory agent (NSAID) and to methods of preparing such compns. The PSA conjugate comprises an oligopeptide that is selectively cleaved by PSA and a cytotoxic agent. An example of a PSA conjugate is N-Ac-(4-trans-L-Hyp)-

Ala-Ser-Chg-Gln-Ser-Leu-Dox (Dox = doxorubicin, Hyp = hydroxyproline, Chg = cyclohexylglycine) and COX-2 inhibitor 3-phenyl-4-[4-(4-methylsulfonyl)phenyl]-2(5H)furanone is an example of an NSAID compound (syntheses given).

IT **189955-00-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(treatment of cancer with prostate specific antigen (PSA) conjugate and NSAID compound)

RN 189955-00-8 HCAPLUS

CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)



L13 ANSWER 13 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:860680 HCAPLUS

DOCUMENT NUMBER: 134:157196

TITLE: Synthesis and analgesic activity of some quinazoline analogs of anpirtoline

AUTHOR(S): Radl, Stanislav; Hezky, Petr; Proska, Jan; Krejci, Ivan

CORPORATE SOURCE: Research Institute of Pharmacy and Biochemistry, Prague, 13060, Czech Rep.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(11), 381-386
CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

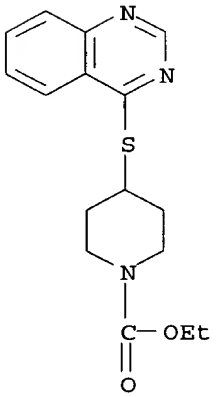
OTHER SOURCE(S): CASREACT 134:157196

AB New condensed derivs. of anpirtoline, in which the pyridine ring is replaced with quinoline, quinazoline, 7-chloroquinoline, and 7-chloroquinazoline nuclei, have been synthesized. Their receptor binding profiles (5-HT1A, 5-HT1B) and analgesic activity (hot plate, acetic acid induced writhing) have been studied. The analgesic activity of some of the compds. are comparable to that of clin. used drugs flupirtine and tramadol under the same conditions.

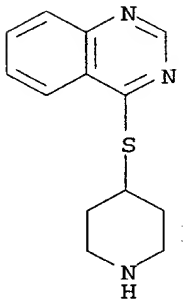
IT **232618-27-8P 232618-31-4P 232618-36-9P**
325145-97-9P 325145-98-0P 325145-99-1P
325146-00-7P 325146-01-8P 325146-02-9P
325146-03-0P 325146-04-1P 325146-05-2P
325146-06-3P 325146-07-4P 325146-08-5P
325146-09-6P 325146-10-9P 325146-11-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and analgesic activity of quinazoline analogs of anpirtoline)

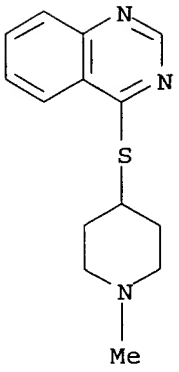
RN 232618-27-8 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinylthio)-, ethyl ester (9CI) (CA INDEX NAME)



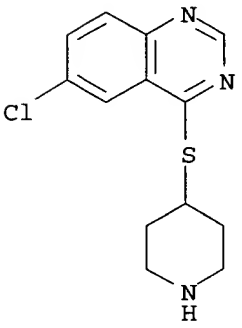
RN 232618-31-4 HCAPLUS
CN Quinazoline, 4-(4-piperidinylthio)- (9CI) (CA INDEX NAME)



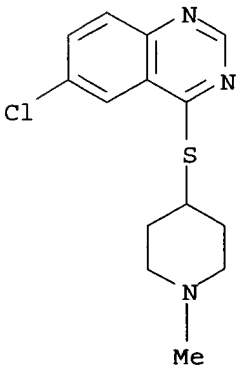
RN 232618-36-9 HCAPLUS
CN Quinazoline, 4-[(1-methyl-4-piperidinyl)thio]- (9CI) (CA INDEX NAME)



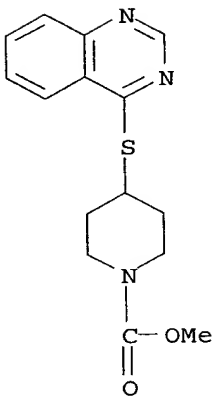
RN 325145-97-9 HCAPLUS
CN Quinazoline, 6-chloro-4-(4-piperidinylthio)- (9CI) (CA INDEX NAME)



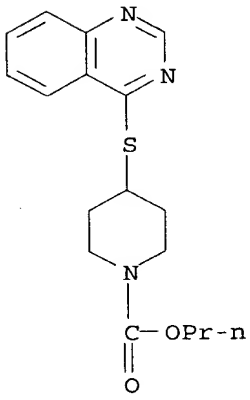
RN 325145-98-0 HCAPLUS
CN Quinazoline, 6-chloro-4-[(1-methyl-4-piperidinyl)thio]- (9CI) (CA INDEX NAME)



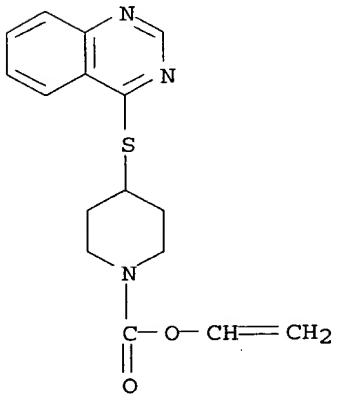
RN 325145-99-1 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinylthio)-, methyl ester (9CI) (CA INDEX NAME)



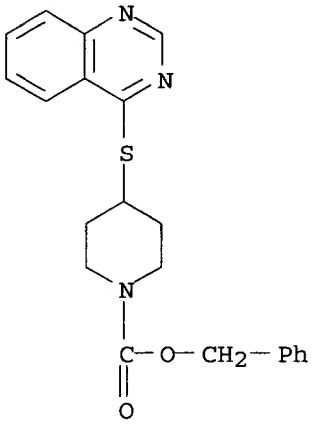
RN 325146-00-7 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinylthio)-, propyl ester (9CI) (CA INDEX NAME)



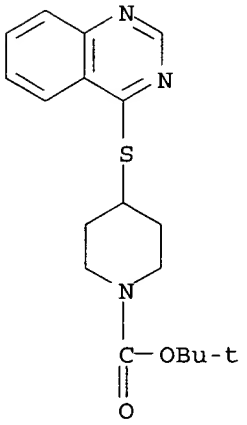
RN 325146-01-8 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinylthio)-, ethenyl ester (9CI) (CA INDEX NAME)



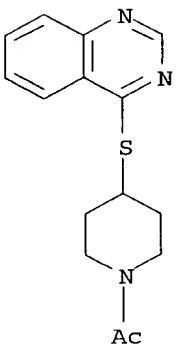
RN 325146-02-9 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinylthio)-, phenylmethyl ester (9CI) (CA INDEX NAME)



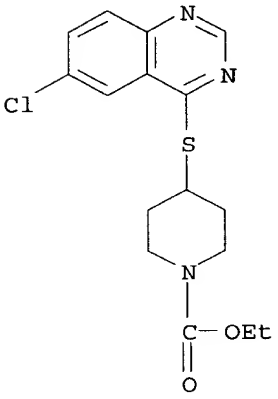
RN 325146-03-0 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinylthio)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



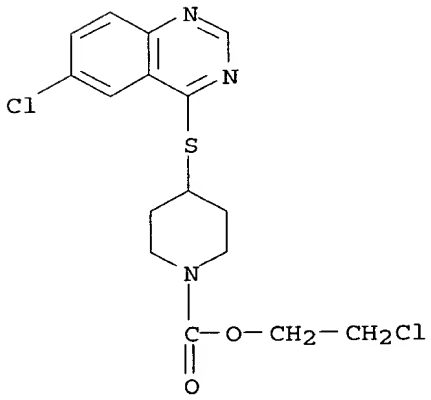
RN 325146-04-1 HCAPLUS
CN Piperidine, 1-acetyl-4-(4-quinazolinylthio)- (9CI) (CA INDEX NAME)



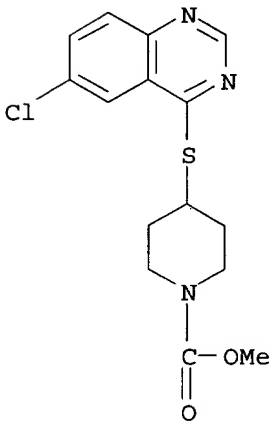
RN 325146-05-2 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[(6-chloro-4-quinazolinyl)thio]-, ethyl ester (9CI) (CA INDEX NAME)



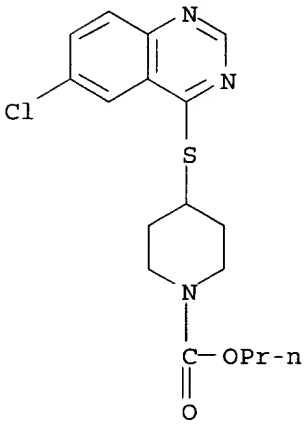
RN 325146-06-3 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[(6-chloro-4-quinazolinyl)thio]-, 2-chloroethyl ester (9CI) (CA INDEX NAME)



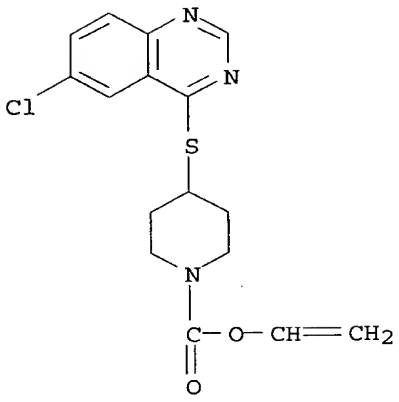
RN 325146-07-4 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[(6-chloro-4-quinazolinyl)thio]-, methyl ester (9CI) (CA INDEX NAME)



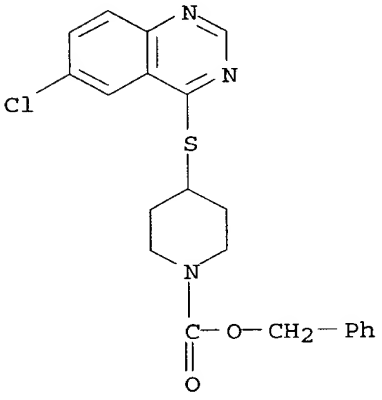
RN 325146-08-5 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[(6-chloro-4-quinazolinyl)thio]-, propyl ester (9CI) (CA INDEX NAME)



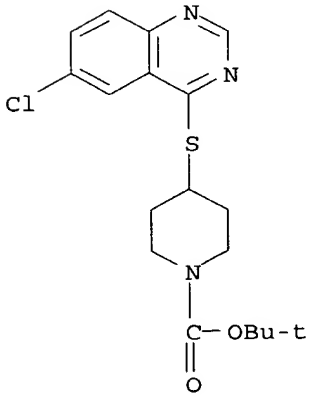
RN 325146-09-6 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[(6-chloro-4-quinazolinyl)thio]-, ethenyl ester (9CI) (CA INDEX NAME)



RN 325146-10-9 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[(6-chloro-4-quinazolinyl)thio]-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 325146-11-0 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-[(6-chloro-4-quinazolinyl)thio]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

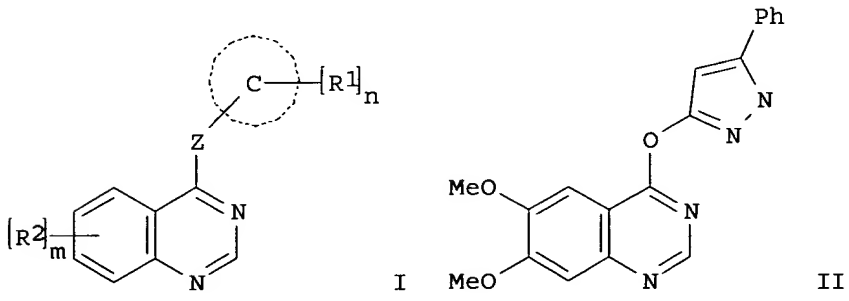


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 14 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:260277 HCAPLUS
DOCUMENT NUMBER: 132:293771
TITLE: Preparation of quinazolines as VEGF receptor tyrosine kinase inhibitors
INVENTOR(S): Hennequin, Laurent Francois Andre; Pasquet, Georges
PATENT ASSIGNEE(S): Zeneca Limited, UK; Zeneca-Pharma S.A.
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000021955	A1	20000420	WO 1999-GB3295		19991005
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2344290	AA	20000420	CA 1999-2344290		19991005
AU 9961128	A1	20000501	AU 1999-61128		19991005
AU 756556	B2	20030116			
BR 9914326	A	20010626	BR 1999-14326		19991005
EP 1119567	A1	20010801	EP 1999-947758		19991005
EP 1119567	B1	20050504			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2002527436	T2	20020827	JP 2000-575861		19991005
NZ 510434	A	20031031	NZ 1999-510434		19991005
AT 294796	E	20050515	AT 1999-947758		19991005
ZA 2001002655	A	20020930	ZA 2001-2655		20010330
NO 2001001739	A	20010607	NO 2001-1739		20010406
PRIORITY APPLN. INFO.:			EP 1998-402496	A	19981008
			WO 1999-GB3295	W	19991005

OTHER SOURCE(S): MARPAT 132:293771
GI

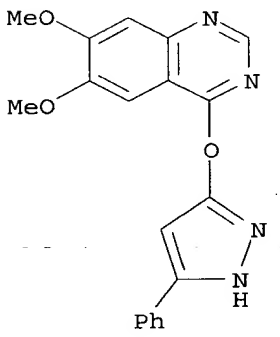


AB The title compds. [I; ring C = 5-6 membered heterocyclic moiety; Z = O, NH, S, CH2; R1 = H, alkyl, alkoxymethyl, etc.; n = 0-5; m = 0-3; R2 = H, OH, halo, etc.] and their salts which inhibit the effects of VEGF , and therefore useful in the production of an antiangiogenic and/or vascular permeability reducing effect in warm-blooded animals, were prepared and formulated. E.g., a multi-step synthesis of quinazoline II was given. Compds. I are effective at 1-50 mg/kg/day.

IT **264207-46-7P 264207-48-9P 264207-50-3P**
264207-52-5P 264207-54-7P 264207-56-9P
264207-58-1P 264207-60-5P 264207-62-7P
264207-64-9P 264207-66-1P 264207-68-3P
264207-70-7P 264207-72-9P 264207-74-1P
264207-76-3P 264207-94-5P 264207-96-7P
264207-98-9P 264208-00-6P 264208-02-8P
264208-04-0P 264208-06-2P 264208-08-4P
264208-10-8P 264208-12-0P 264208-14-2P
264208-16-4P 264208-18-6P 264208-21-1P
264208-23-3P 264208-26-6P 264208-28-8P
264208-31-3P 264208-33-5P 264208-35-7P
264208-38-0P 264208-41-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinazolines as VEGF receptor tyrosine kinase inhibitors)

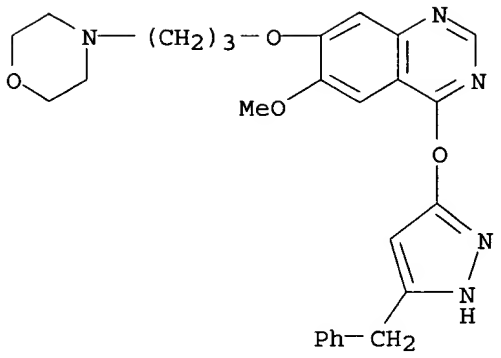
RN 264207-46-7 HCAPLUS

CN Quinazoline, 6,7-dimethoxy-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]- (9CI) (CA INDEX NAME)

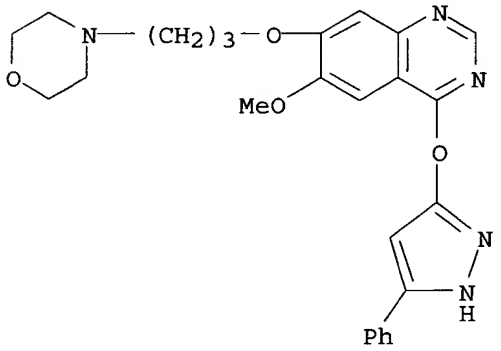


RN 264207-48-9 HCAPLUS

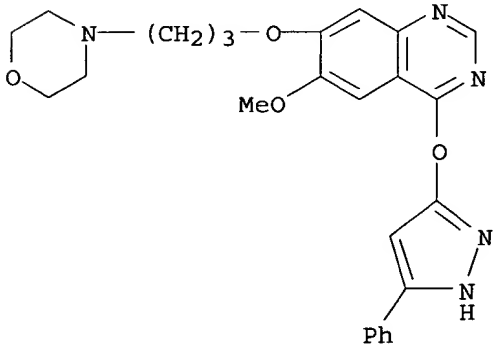
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[5-(phenylmethyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



RN 264207-50-3 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]- (9CI) (CA INDEX NAME)

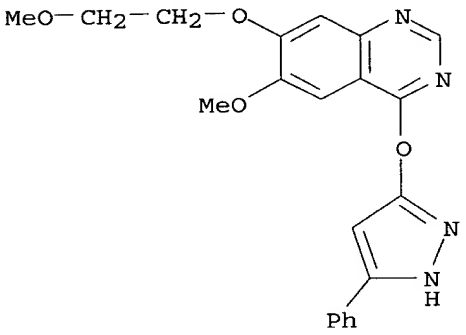


RN 264207-52-5 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

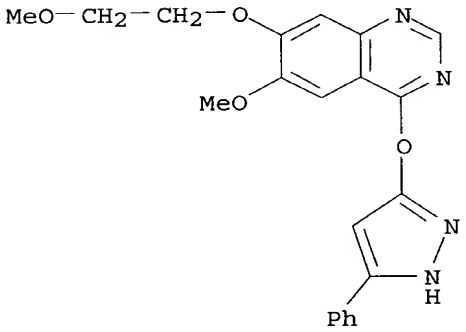


●2 HCl

RN 264207-54-7 HCAPLUS
CN Quinazoline, 6-methoxy-7-(2-methoxyethoxy)-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]- (9CI) (CA INDEX NAME)

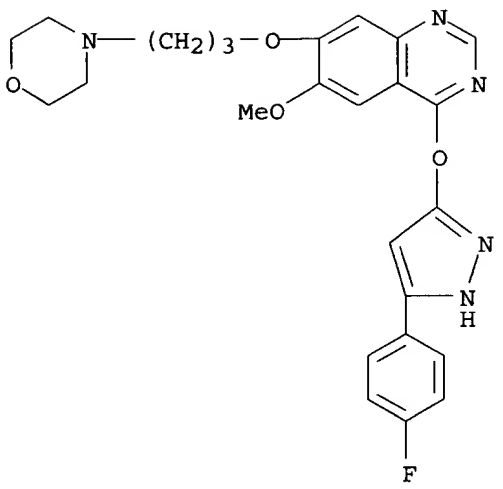


RN 264207-56-9 HCAPLUS
CN Quinazoline, 6-methoxy-7-(2-methoxyethoxy)-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]-, hydrochloride (4:3) (9CI) (CA INDEX NAME)



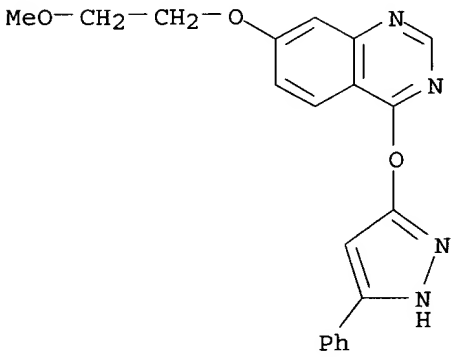
● 3/4 HCl

RN 264207-58-1 HCAPLUS
CN Quinazoline, 4-[[5-(4-fluorophenyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]-, hydrochloride (10:19) (9CI) (CA INDEX NAME)



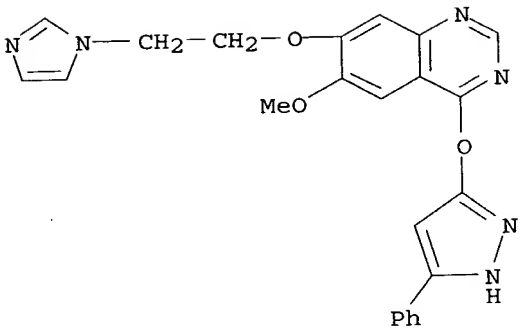
●19/10 HCl

RN 264207-60-5 HCAPLUS
CN Quinazoline, 7-(2-methoxyethoxy)-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]-, hydrochloride (5:3) (9CI) (CA INDEX NAME)



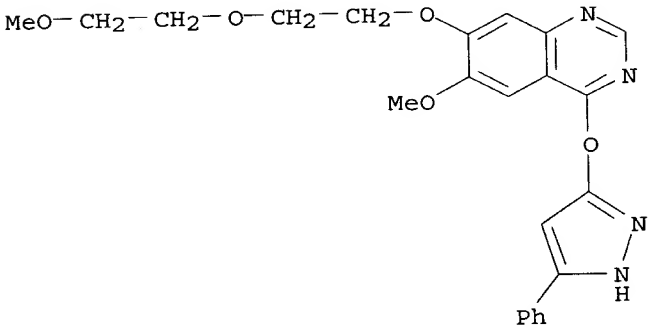
●3/5 HCl

RN 264207-62-7 HCAPLUS
CN Quinazoline, 7-[2-(1H-imidazol-1-yl)ethoxy]-6-methoxy-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]-, hydrochloride (2:5) (9CI) (CA INDEX NAME)



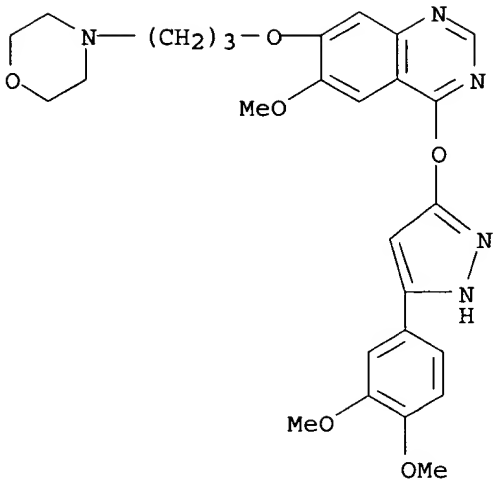
●5/2 HCl

RN 264207-64-9 HCAPLUS
CN Quinazoline, 6-methoxy-7-[2-(2-methoxyethoxy)ethoxy]-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]-, hydrochloride (20:17) (9CI) (CA INDEX NAME)

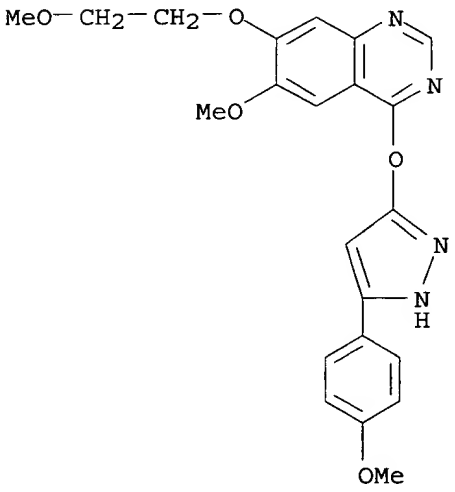


●17/20 HCl

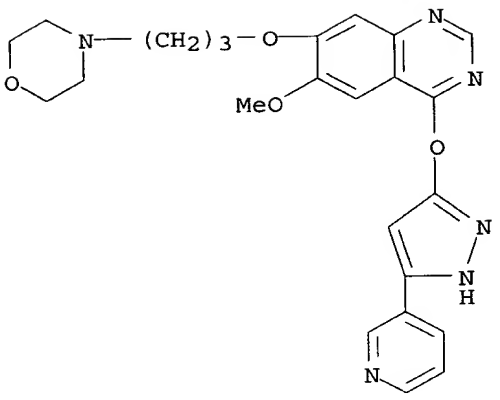
RN 264207-66-1 HCAPLUS
CN Quinazoline, 4-[[5-(3,4-dimethoxyphenyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



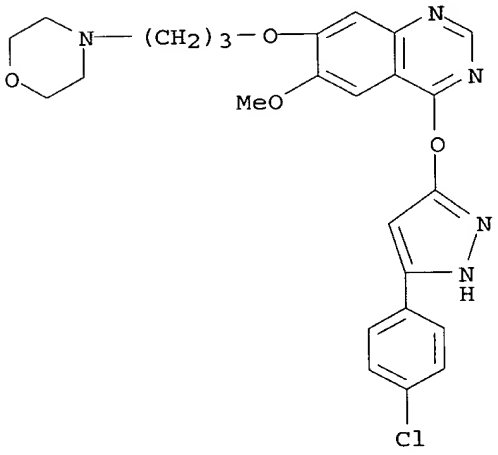
RN 264207-68-3 HCAPLUS
CN Quinazoline, 6-methoxy-7-(2-methoxyethoxy)-4-[[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



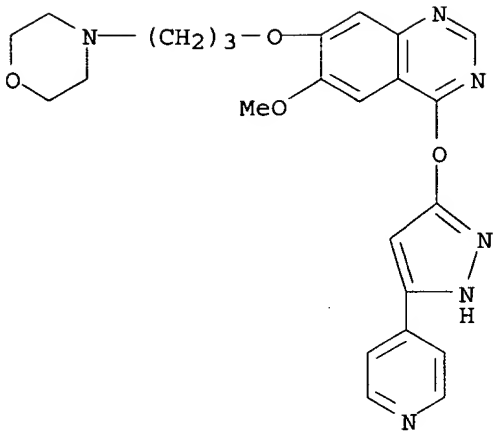
RN 264207-70-7 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[5-(3-pyridinyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



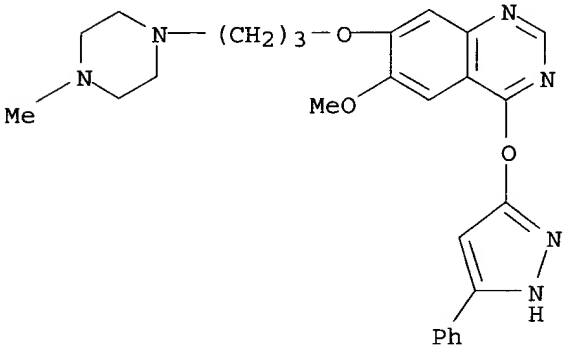
RN 264207-72-9 HCAPLUS
CN Quinazoline, 4-[[5-(4-chlorophenyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



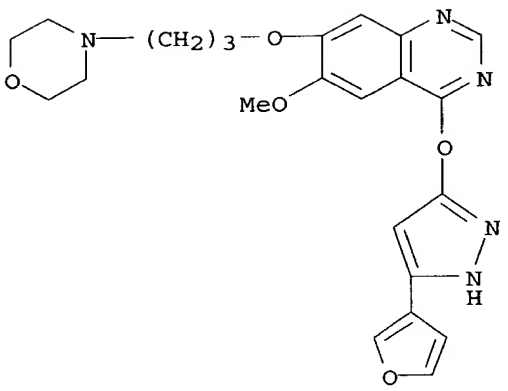
RN 264207-74-1 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[5-(4-pyridinyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



RN 264207-76-3 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-methyl-1-piperazinyl)propoxy]-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]- (9CI) (CA INDEX NAME)

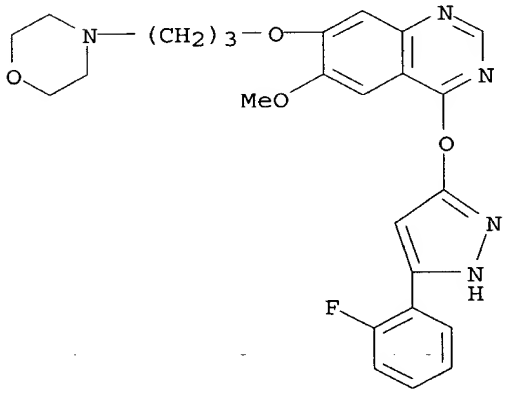


RN 264207-94-5 HCAPLUS
CN Quinazoline, 4-[[5-(3-furanyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]-, hydrochloride (9CI) (CA INDEX NAME)

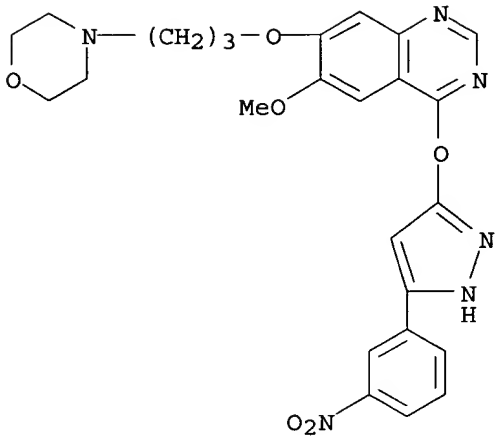


●x HCl

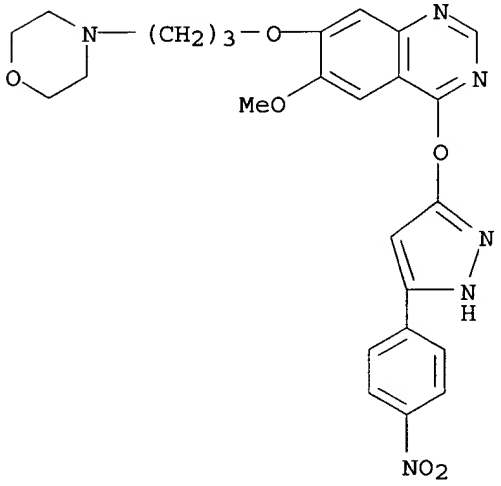
RN 264207-96-7 HCAPLUS
CN Quinazoline, 4-[[5-(2-fluorophenyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



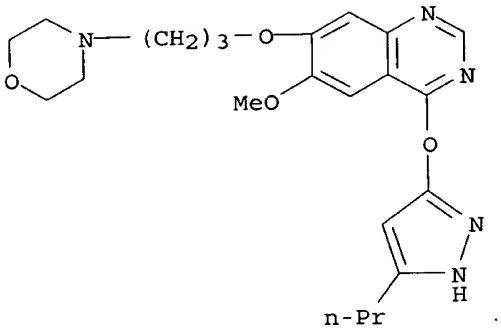
RN 264207-98-9 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[5-(3-nitrophenyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



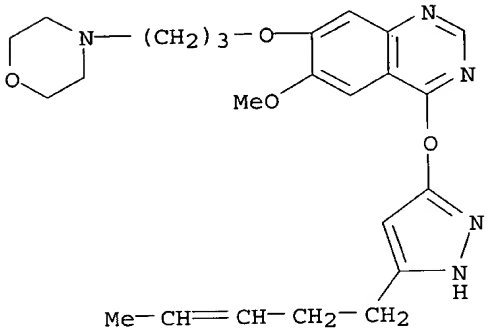
RN 264208-00-6 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[5-(4-nitrophenyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



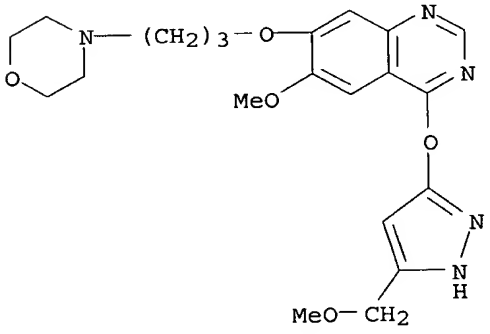
RN 264208-02-8 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[(5-propyl-1H-pyrazol-3-yl)oxy]- (9CI) (CA INDEX NAME)



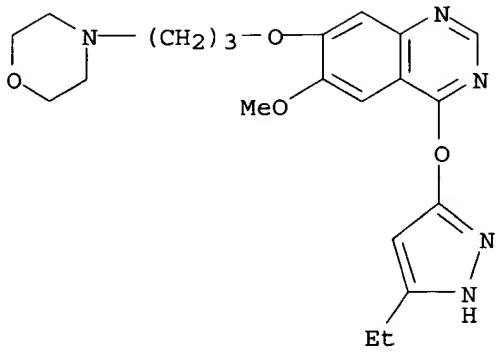
RN 264208-04-0 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[5-(3-pentenyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



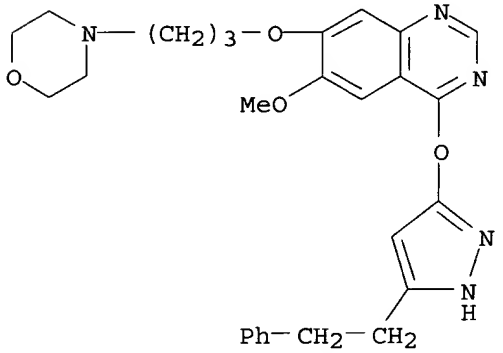
RN 264208-06-2 HCAPLUS
CN Quinazoline, 6-methoxy-4-[[5-(methoxymethyl)-1H-pyrazol-3-yl]oxy]-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



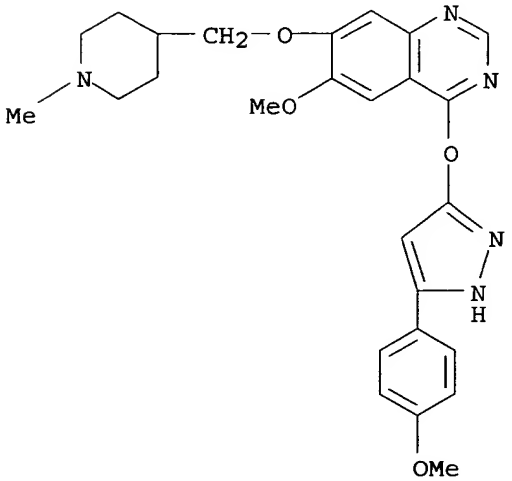
RN 264208-08-4 HCAPLUS
CN Quinazoline, 4-[(5-ethyl-1H-pyrazol-3-yl)oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



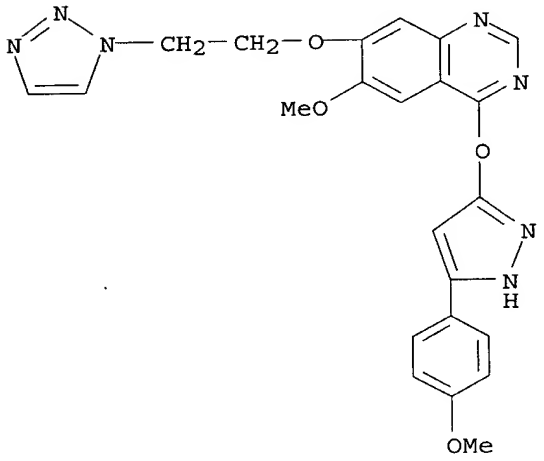
RN 264208-10-8 HCAPLUS
CN Quinazoline, 6-methoxy-7-[3-(4-morpholinyl)propoxy]-4-[[5-(2-phenylethyl)-1H-pyrazol-3-yl]oxy]- (9CI) (CA INDEX NAME)



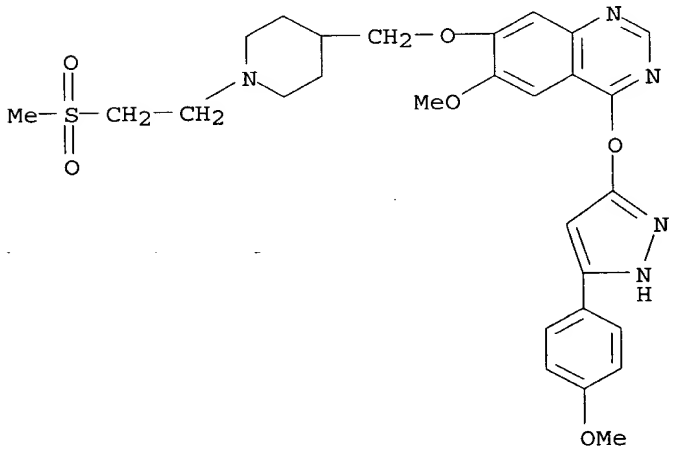
RN 264208-12-0 HCAPLUS
CN Quinazoline, 6-methoxy-4-[[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]oxy]-7-[(1-methyl-4-piperidinyl)methoxy]- (9CI) (CA INDEX NAME)



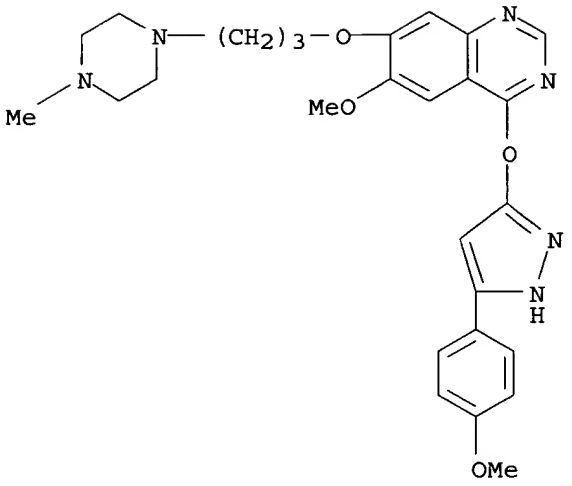
RN 264208-14-2 HCAPLUS
CN Quinazoline, 6-methoxy-4-[[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]oxy]-7-[2-(1H-1,2,3-triazol-1-yl)ethoxy]- (9CI) (CA INDEX NAME)



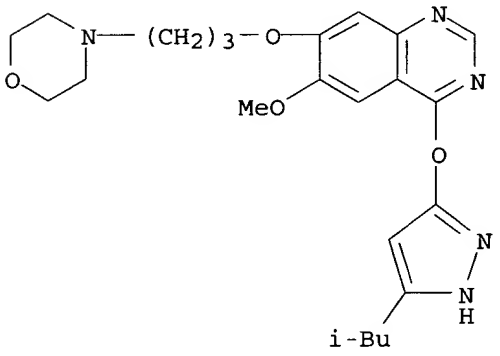
RN 264208-16-4 HCAPLUS
CN Quinazoline, 6-methoxy-4-[[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]oxy]-7-[[1-[2-(methylsulfonyl)ethyl]-4-piperidinyl]methoxy]- (9CI) (CA INDEX NAME)



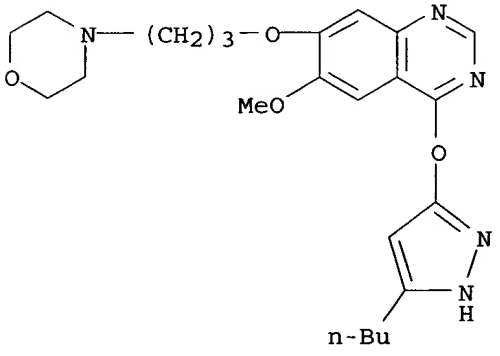
RN 264208-18-6 HCAPLUS
CN Quinazoline, 6-methoxy-4-[[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]oxy]-7-[3-(4-methyl-1-piperazinyl)propoxy]- (9CI) (CA INDEX NAME)



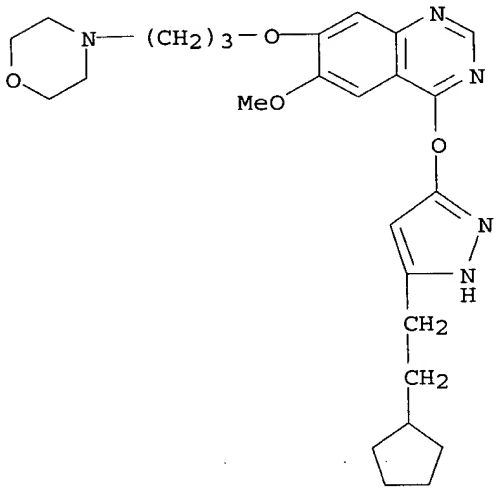
RN 264208-21-1 HCAPLUS
CN Quinazoline, 6-methoxy-4-[[5-(2-methylpropyl)-1H-pyrazol-3-yl]oxy]-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



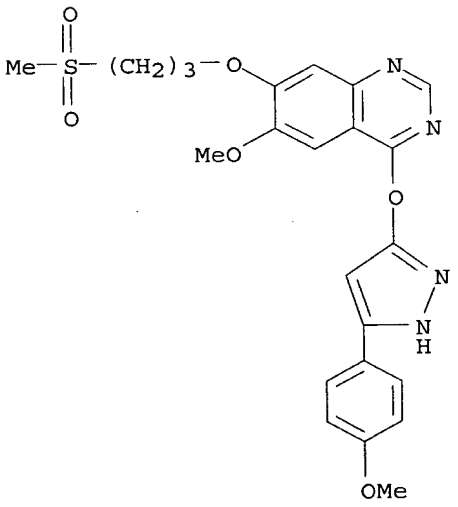
RN 264208-23-3 HCAPLUS
CN Quinazoline, 4-[(5-butyl-1H-pyrazol-3-yl)oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



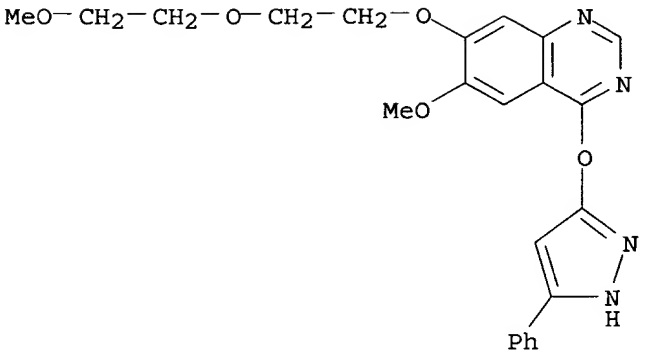
RN 264208-26-6 HCAPLUS
CN Quinazoline, 4-[[5-(2-cyclopentylethyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



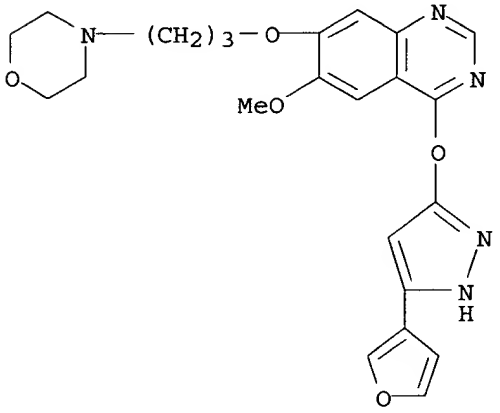
RN 264208-28-8 HCAPLUS
CN Quinazoline, 6-methoxy-4-[[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]oxy]-7-[3-(methylsulfonyl)propoxy]- (9CI) (CA INDEX NAME)



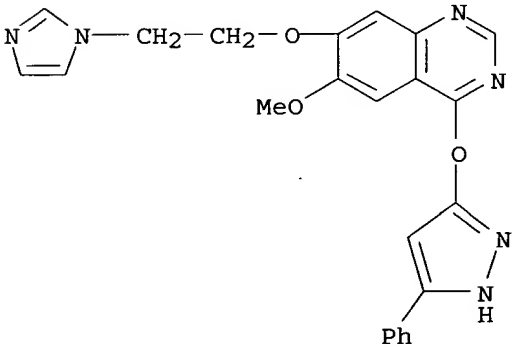
RN 264208-31-3 HCAPLUS
CN Quinazoline, 6-methoxy-7-[2-(2-methoxyethoxy)ethoxy]-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]- (9CI) (CA INDEX NAME)



RN 264208-33-5 HCAPLUS
CN Quinazoline, 4-[[5-(3-furanyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)

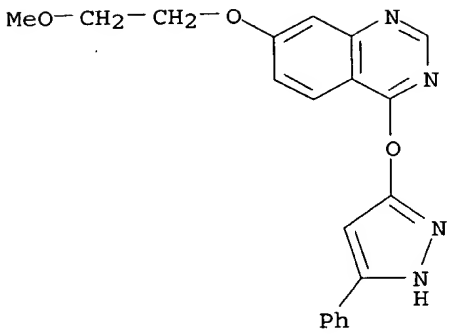


RN 264208-35-7 HCAPLUS
CN Quinazoline, 7-[2-(1H-imidazol-1-yl)ethoxy]-6-methoxy-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]- (9CI) (CA INDEX NAME)

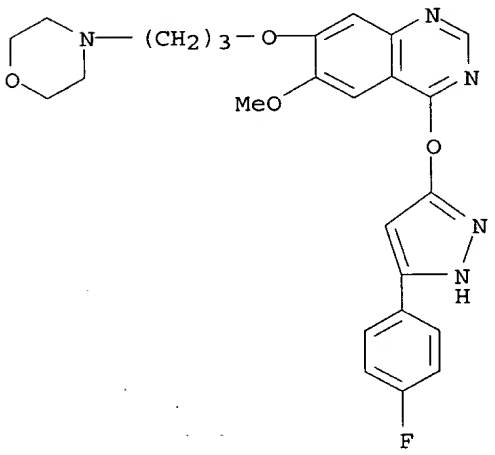


RN 264208-38-0 HCAPLUS
CN Quinazoline, 7-(2-methoxyethoxy)-4-[(5-phenyl-1H-pyrazol-3-yl)oxy]- (9CI)

(CA INDEX NAME)



RN 264208-41-5 HCAPLUS
CN Quinazoline, 4-[[5-(4-fluorophenyl)-1H-pyrazol-3-yl]oxy]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



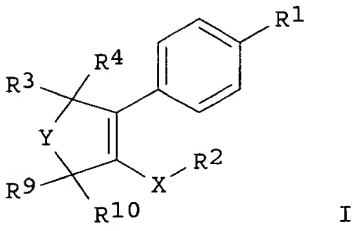
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 15 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:83114 HCAPLUS
DOCUMENT NUMBER: 132:122509
TITLE: Preparation of (methylsulfonyl)phenyl-2-(5H)-furanones as COX-2 inhibitors
INVENTOR(S): Belley, Michel; Gauthier, Jacques Yves; Grimm, Erich; Leblanc, Yves; Li, Chun-sing; Therien, Michel; Black, Cameron; Prasit, Petpiboon; Lau, Cheuk-kun; Roy, Patrick
PATENT ASSIGNEE(S): Merck Frosst Canada, Inc., Can.
SOURCE: U.S., 88 pp., Cont.-in-part of U.S. Ser. No. 728,512, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 6020343	A	20000201	US 1998-97543		19980615
NZ 332820	A	20000526	NZ 1996-332820		19961009
JP 2001199954	A2	20010724	JP 2000-366579		19961009
ZA 9608609	A	19970414	ZA 1996-8609		19961011
US 6169188	B1	20010102	US 1999-422151		19991021
PRIORITY APPLN. INFO.:			US 1995-5371P	P	19951013
			US 1996-11637P	P	19960214
			US 1996-728512	B2	19961009
			GB 1996-2939	A	19960213
			GB 1996-5645	A	19960318
			JP 1997-515371	A3	19961009
			NZ 1996-319090	A1	19961009
			US 1998-97543	A3	19980615

OTHER SOURCE(S): MARPAT 132:122509
GI



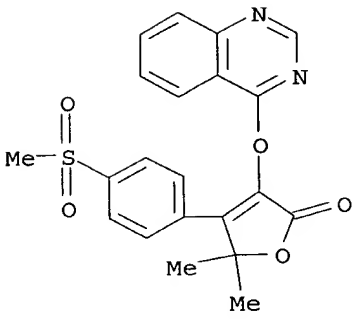
I

AB The title compds. [I; X = CH2, CHOH, CO, etc.; Y = O, S, CO, etc.; R1 = SO2Me, SO2NHCOCF3, SONHNH2, etc.; R2 = alkyl, (un)substituted Ph, naphthyl, etc.; R3 = H, alkyl, CN, etc.; R4 = H, alkyl, alkoxy, etc.; R9, R10 = H, alkyl; R9 and R10 together with the carbon atom to which they are attached form a carbonyl or thiocarbonyl group], useful in the treatment of cyclooxygenase-2 mediated diseases such as inflammation, arthritis, osteoporosis, rheumatoid arthritis, and pain, were prepared E.g., a 4-step synthesis of I [X = O; Y = O; R1 = SO2Me; R2 = 3,4-F2C6H3; R3 = R4 = Me; R9 and R10 together with the carbon atom to which they are attached form a carbonyl group] which showed ED50 of 0.14 mg/kg in rat paw edema assay, was given.

IT **189955-00-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (methylsulfonyl)phenyl-2-(5H)-furanones as COX-2 inhibitors)

RN 189955-00-8 HCAPLUS

CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)



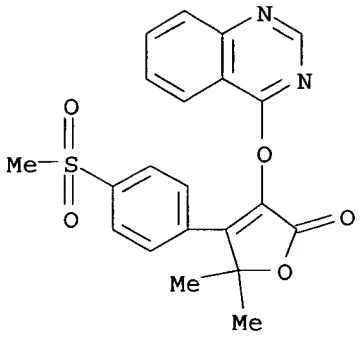
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 16 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:769077 HCAPLUS
DOCUMENT NUMBER: 132:73232
TITLE: Synthesis and biological evaluation of 3-heteroaryloxy-4-phenyl-2(5H)-furanones as selective COX-2 inhibitors
AUTHOR(S): Lau, Cheuk K.; Brideau, Christine; Chan, Chi Chung; Charleson, Stella; Cromlish, Wanda A.; Ethier, Diane; Gauthier, Jacques Yves; Gordon, Robert; Guay, Jocelyne; Kargman, Stacia; Li, Chun-Sing; Prasit, Petpiboon; Riendeau, Denis; Therien, Michel; Visco, Denise M.; Xu, Lijing
CORPORATE SOURCE: Merck Frosst Centre for Therapeutic Research, Pointe Claire-Dorval, QC, H9R 4P8, Can.
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(22), 3187-3192
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of 3-heteroaryloxy-4-phenyl-2-(5H)-furanones were prepared and evaluated for their potency and selectivity as COX-2 inhibitors. This led to the identification of L-778,736 as a potent, orally active and selective inhibitor of the COX-2 enzyme.

IT **189955-00-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-anti-inflammatory activity of cyclooxygenase 2 inhibitors heteroaryloxyphenylfuranones)

RN 189955-00-8 HCAPLUS
CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)

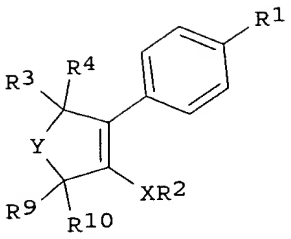


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 17 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:718982 HCAPLUS
DOCUMENT NUMBER: 131:322532
TITLE: Preparation of 4-aryl-(5H)-furan-2-ones as cyclooxygenase-2 inhibitors.
INVENTOR(S): Belley, Michel; Gauthier, Jacques Yves; Grimm, Erich; Leblanc, Yves; Li, Chun-Sing; Therien, Michel; Black, Cameron; Prasit, Petpiboon; Lau, Cheuk-Kun; Roy, Patrick
PATENT ASSIGNEE(S): Merck Frosst Canada, Inc., Can.
SOURCE: U.S., 74 pp., Cont.-in-part of U.S. Ser. No. 728,512, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 5981576	A	19991109	US 1998-97537		19980615
NZ 332820	A	20000526	NZ 1996-332820		19961009
JP 2001199954	A2	20010724	JP 2000-366579		19961009
ZA 9608609	A	19970414	ZA 1996-8609		19961011
PRIORITY APPLN. INFO.:			US 1995-5371P	P	19951013
			US 1996-11637P	P	19960214
			US 1996-728512	B2	19961009
			GB 1996-2939	A	19960213
			GB 1996-5645	A	19960318
			JP 1997-515371	A3	19961009
			NZ 1996-319090	A1	19961009

OTHER SOURCE(S): MARPAT 131:322532
GI



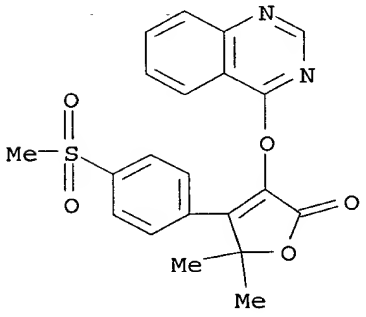
I

AB Title compds. [I; X = CH2, CH(OH), CO, O, S, NR15; Y = CO, O, S, CR11R12; R1 = SO2Me, SO2NR16R17, SO2NHCOCF3, etc.; R2 = alkyl, (substituted) Ph, naphthyl, heteroaryl, benzoheterocyclyl, heterocyclylalkyl, benzocarbocyclyl, etc.; R3 = H, alkyl, CH2OR7, cyano, CH2CN, (substituted) Ph, etc.; R4 = H, alkyl, alkoxy, alkylthio, OH, SH, OCOR7, etc.; R3R4 = atoms to form a 3-7 membered ring; R7 = H, alkyl, (substituted) Ph, PhCH2; R9, R10 = H, alkyl; R9R10 = O, S; R16, R17 = H, alkyl, alkanoic acid, alkyl amine, etc.; with provisos], were prepared Thus, cyclopropanemethanol in THF was added to NaH in THF at 12° over 75 min. followed by 18 h stirring at room temperature; ClCH2CO2Na was added followed by 8.5 h reflux to give an oil. This was refluxed with 2-bromo-2-methyl-1-[(4-methylsulfonyl)phenyl]propan-1-one (preparation given) and ethyldiisopropylamine in EtOH to give cyclopropylmethoxyacetic acid 2-methyl-1-[(4-methylsulfonyl)phenyl]propan-1-one ester. The latter was refluxed with iso-Pr trifluoroacetate and DBU in MeCN to give 3-(cyclopropylmethoxy)-5,5-dimethyl-4-[(4-methylsulfonyl)phenyl]-5H-furan-2-one. I inhibited rat paw edema with ED50 = 0.32-10 mg/kg orally.

IT **189955-00-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-aryl-(5H)-furan-2-ones as cyclooxygenase-2 inhibitors)

RN 189955-00-8 HCAPLUS

CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

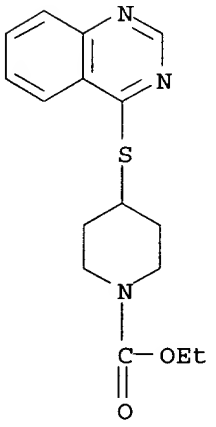
L13 ANSWER 18 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:410148 HCAPLUS
DOCUMENT NUMBER: 131:111116

TITLE: Synthesis and analgesic activity of some condensed analogs of anpirtoline
AUTHOR(S): Radl, Stanislav; Kovarova, Lenka; Hezky, Petr; Vosatka, Vaclav; Konigova, Otylie; Proska, Jan; Krejci, Ivan
CORPORATE SOURCE: Research Institute Pharmacy Biochemistry, Prague, 13060, Czech Rep.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1999), 332(6), 208-212
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Condensed derivs. of anpirtoline, in which the pyridine ring is replaced with quinoline, isoquinoline, quinazoline, and phthalazine nuclei, were synthesized. Their receptor binding profiles (5HT1A, 5-HT1B) and analgesic activity (hot plate, AcOH-induced writhing) were studied. The analgesic activity of 4 of the compds. are at least comparable to that of the clin. used drugs flupirtine and tramadol under the same conditions.

IT **232618-27-8P 232618-32-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and 5-HT1-agonistic and analgesic activity of condensed analogs of anpirtoline)

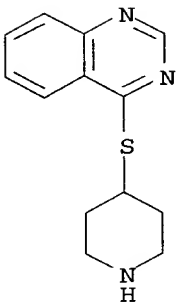
RN 232618-27-8 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(4-quinazolinylthio)-, ethyl ester (9CI) (CA INDEX NAME)



RN 232618-32-5 HCAPLUS
CN Quinazoline, 4-(4-piperidinylthio)-, monoacetate (9CI) (CA INDEX NAME)

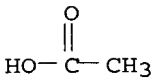
CM 1

CRN 232618-31-4
CMF C13 H15 N3 S

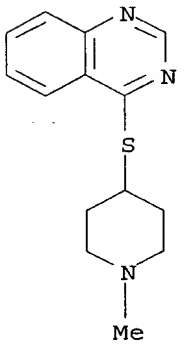


CM 2

CRN 64-19-7
CMF C2 H4 O2



IT **232618-36-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and 5-HT1-agonistic and analgesic activity of condensed analogs of anpirtoline)
RN 232618-36-9 HCAPLUS
CN Quinazoline, 4-[(1-methyl-4-piperidinyl)thio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 19 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:425272 HCAPLUS
DOCUMENT NUMBER: 127:34112
TITLE: Preparation of 3,4-diaryl-2-hydroxy-2,5-dihydrofurans as prodrugs to cyclooxygenase-2 (cox-2) inhibitors and as non-steroidal anti-inflammatory agents

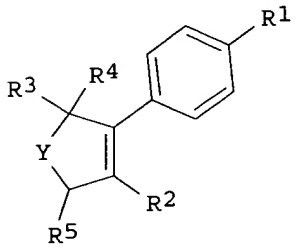
INVENTOR(S): Black, Cameron; Leger, Serge; Prasit, Petpiboon; Wang, Zhaoyin; Hamel, Pierre; Han, Yongxin; Hughes, Gregory
PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.
SOURCE: PCT Int. Appl., 213 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 9
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9716435	A1	19970509	WO 1996-CA717	19961029
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5698584	A	19971216	US 1996-738143	19961025
CA 2234642	AA	19970509	CA 1996-2234642	19961029
CA 2234642	C	20050726		
AU 9672736	A1	19970522	AU 1996-72736	19961029
AU 711902	B2	19991021		
JP 11500748	T2	19990119	JP 1997-516943	19961029
JP 3337477	B2	20021021		
EP 904269	A1	19990331	EP 1996-934267	19961029
EP 904269	B1	20020123		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, LI, LU, NL, SE, PT, IE, FI				
AT 212343	E	20020215	AT 1996-934267	19961029
ES 2171723	T3	20020916	ES 1996-934267	19961029
US 6057319	A	20000502	US 1998-68139	19981002

PRIORITY APPLN. INFO.:

US 1995-8074P	P	19951030
GB 1996-2877	A	19960213
WO 1996-CA717	W	19961029

OTHER SOURCE(S): MARPAT 127:34112
GI



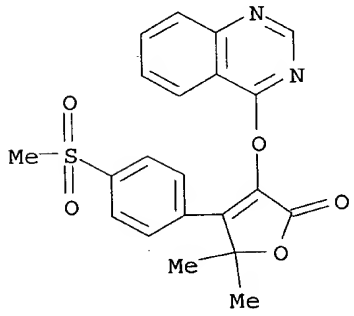
I

AB The invention encompasses the novel compound of formula [I; Y = (un)substituted CH2, O, S, CO; R2 = SO2Me, (un)substituted SO2NH2, SO2NHCOCF3, SONHNH2, SONHNHCOCF3, P(O)MeNH2, P(O)Me2, C(S)NH2; R2 = NR10R11, SR11, OR11, R11, C1-10 alkenyl, C1-10 alkynyl, (un)substituted C3-10 cycloalkenyl; wherein R11 = C1-10 alkyl, C3-10 cycloalkyl, (un)substituted Ph, naphthyl, or heteroaryl, etc.; R3 = H, C1-10 alkyl, cyano, CH2CN, C1-6 fluoroalkyl, F, CH2OR8, CON(R8)2; R4 = H, C1-10 alkyl,

C1-10 alkoxy, C1-10 alkylthio, OH, O2CR8, SH, SCOR8, OCO2R8, O CON(R8)2, SCON(R8)2, C3-10 cycloalkoxy or cycloalkylthio; or CR3R4 = 3- to 7-membered monocyclic ring optionally containing 1 or 2 heteroatoms selected from O, S, or N; wherein R8 = H, C1-10 alkyl, C1-10 alkyl-CO2H, C1-10 aminoalkyl, (un)substituted Ph or CH2Ph, C3-10 cycloalkyl, C1-10 alkanoyl, (un)substituted benzoyl; R5 = OR17, SR18, NR17R18, S(O)R18, SO2 R18, SO2N(R17)2, OP(O)(OR16)2; wherein R16 = H, C1-6 alkyl, (un)substituted CH2Ph; R17 = H, R18; R18 = C1-10 alkyl, C1-10 alkyl-CO2H, C1-10 aminoalkyl, (un)substituted Ph or CH2Ph, C3-10 cycloalkyl, (CH2CH2O)nH (n = 1-6), C1-10 alkanoyl, (un)substituted benzoyl]. They are in vivo converted into the active lactone form, i.e. arylhydroxydihydrofuranone derivs. I (R5 = oxo; Y, R1 - R4 = same as above) with high inhibitory activity against cyclooxygenase-2 and/or a specificity for cyclooxygenase-2 over cyclooxygenase-1 and useful in the treatment of cyclooxygenase-2 mediated diseases, in particular inflammatory diseases. Thus, 3,4-difluorophenoxyacetic acid was cyclocondensed with 2-hydroxy-4'-(methylsulfonyl)isobutyrophenone (preparation given) using 1-cyclohexyl-3-(2-morpholinoethyl)carbodiimide metho-p-toluenesulfonate and 4-dimethylaminopyridine in CH2Cl2 at room temperature for 18 h to give 3-(3,4-difluorophenoxy)-5,5-dimethyl-4-(4-methylsulfonylphenyl)-5H-furan-2-one, which was reduced by (Me2CHCH2)2AlH in THF at room temperature for 30 min to give I (Y = O, R2 = 3,4-difluorophenoxy, R3 = R4 = Me, R5 = OH). The latter compound showed ED50 of 0.09 mg/kg p.o. for inhibiting the carrageenan-induced paw edema in rats.

IT **189955-00-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diarylhydroxydihydrofurans as prodrugs for antiinflammatory diarylhydroxydihydrofuranones and selective cyclooxygenase-2 inhibitors)

RN 189955-00-8 HCAPLUS
CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)



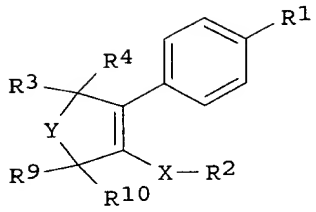
L13 ANSWER 20 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:384238 HCAPLUS
DOCUMENT NUMBER: 127:5002
TITLE: (Methylsulfonyl)phenyl-2-(5H)-furanones as cox-2 inhibitors
INVENTOR(S): Belley, Michel; Gauthier, Jacques Y.; Grimm, Erich; Leblanc, Yves; Li, Chung-Sing; Therien, Michel; Black,

Cameron; Lau, Cheuk-Kun; Prasit, Petpiboon; et al.
PATENT ASSIGNEE(S): Can.
SOURCE: PCT Int. Appl., 264 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9714691	A1	19970424	WO 1996-CA682	19961009
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
HR 960458	B1	20030831	HR 1996-960458	19961007
CA 2233178	AA	19970424	CA 1996-2233178	19961009
CA 2233178	C	20031223		
AU 9671236	A1	19970507	AU 1996-71236	19961009
AU 703871	B2	19990401		
EP 863891	A1	19980916	EP 1996-932417	19961009
EP 863891	B1	20021211		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI				
CN 1200119	A	19981125	CN 1996-197609	19961009
JP 11500146	T2	19990106	JP 1997-515371	19961009
JP 3337476	B2	20021021		
BR 9611015	A	19990914	BR 1996-11015	19961009
NZ 319090	A	20000128	NZ 1996-319090	19961009
NZ 332820	A	20000526	NZ 1996-332820	19961009
JP 2001199954	A2	20010724	JP 2000-366579	19961009
IL 123699	A1	20020310	IL 1996-123699	19961009
SK 282639	B6	20021008	SK 1998-450	19961009
AT 229515	E	20021215	AT 1996-932417	19961009
EE 3969	B1	20030217	EE 1998-80	19961009
PT 863891	T	20030331	PT 1996-932417	19961009
ES 2187675	T3	20030616	ES 1996-932417	19961009
RO 119884	B1	20050530	RO 1998-856	19961009
PL 188918	B1	20050531	PL 1996-326203	19961009
ZA 9608609	A	19970414	ZA 1996-8609	19961011
TW 426679	B	20010321	TW 1996-85112463	19961012
NO 9801628	A	19980527	NO 1998-1628	19980408
BG 63391	B1	20011231	BG 1998-102425	19980504

PRIORITY APPLN. INFO.:		
US 1995-5371P	P	19951013
GB 1996-2939	A	19960213
US 1996-11637P	P	19960214
GB 1996-5645	A	19960318
US 1995-5371	P	19951013
US 1996-11637	P	19960214
JP 1997-515371	A3	19961009
NZ 1996-319090	A1	19961009
WO 1996-CA682	W	19961009

OTHER SOURCE(S): MARPAT 127:5002
GI



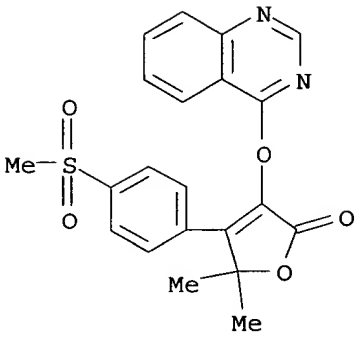
I

AB The title compds. [I; X = CH2, CHOH, CO, O, S, NR15 with the proviso that when R3 and R4 are other than both H, both C1-10 alkyl, or joined together with the carbon to which they are attached to form a saturated monocyclic carbon ring of 3, 4, 5, 6 or 7 atoms, then X is selected from CO, O, S, or NR15; Y = CR11R12, CO, O, S; R11, R12 = H, mono- or disubstituted Ph or mono- or disubstituted benzyl or mono- or disubstituted heteroaryl or mono- or disubstituted heteroarylmethyl wherein the substituents are H, halo, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio, etc.; R1 = SO2-Me, SO2-NR16R17, SO2-NH-CO-CF3, SONH-NH2, etc.; R2 = H, halo, C1-10 alkyl, mono- or disubstituted Ph or naphthyl wherein the substituents are selected from the group consisting of H, halo, C1-10 alkoxy, C1-10 alkylthio, etc.; R3 = H, C1-10 alkyl, CH2-OR7, CN, CH2CN, C1-6 fluoroalkyl, F, etc.; R4 = H, C1-10 alkyl, C1-10 alkoxy, C1-10 alkylthio, OH, etc.; R9, R10 = H, C1-7 alkyl, or R9R10 together with the carbon atom they are attached form a carbonyl or thiocarbonyl group; R15 = H, C1-10 alkyl, mono-, di-, or trisubstituted Ph or naphthyl, etc.; R16, R17 = H, C1-10 alkyl, alkanoic acid, alkyl amine, etc.] are prepared Thus, 2-methyl-1-[4-(methylthio)phenyl]-1-propanone (prepared from isobutyryl chloride and thioanisole) was treated with Aliquat 336 to give the 2-hydroxy derivative, which was oxidized to the sulfonyl compound with Oxone, which was reacted with 3,4-difluorophenoxyacetic acid to give I [R1 = SO2-Me, R2 = 3,4-difluorophenyl, R3 = R4 = Me, R9R10 = O, X = Y = O]. In a red paw edema assay (using rats) for its antiinflammatory potency, this had ED50 of 0.14 mg/Kg. The invention also describes pharmaceutical compns. comprising I for treatment of cyclooxygenase-2 mediated diseases.

IT **189955-00-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
((methylsulfonyl)phenyl(5H)-furanones as cox-2 inhibitors)

RN 189955-00-8 HCAPLUS

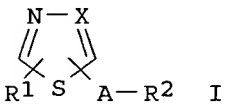
CN 2(5H)-Furanone, 5,5-dimethyl-4-[4-(methylsulfonyl)phenyl]-3-(4-quinazolinyloxy)- (9CI) (CA INDEX NAME)



L13 ANSWER 21 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:708170 HCAPLUS
DOCUMENT NUMBER: 125:328719
TITLE: Preparation of thiazoles and thiadiazoles for treatment of thrombocytopenia
INVENTOR(S): Matsuo, Masaaki; Ogino, Takashi; Tsuji, Kiyoshi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9630370	A2	19961003	WO 1996-JP773		19960326
WO 9630370	A3	19961128			
W: AU, CA, CN, HU, JP, KR, NO, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
ZA 9602398	A	19961001	ZA 1996-2398		19960326
AU 9650153	A1	19961016	AU 1996-50153		19960326
PRIORITY APPLN. INFO.:			GB 1995-6189	A	19950327
			GB 1995-11226	A	19950602
			WO 1996-JP773	W	19960326

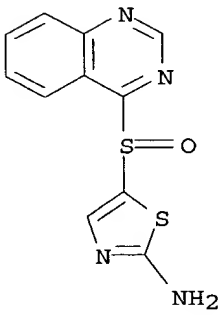
OTHER SOURCE(S): MARPAT 125:328719
GI



I

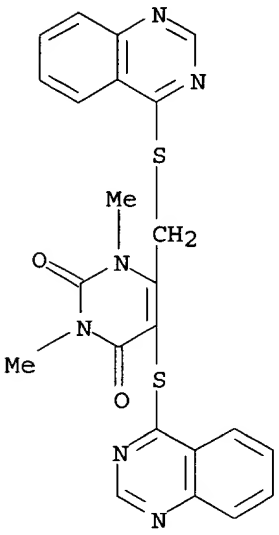
AB The title compds. [I; R1 = H, halo, NH2, etc.; R2 = N- or S-containing unsatd. heterocyclic group; X = CH, N; A = S(O)m (wherein m = 0-2)], useful for prophylactic or therapeutic treatment of thrombocytopenia, rheumatism, nephritis, tumor or side effects of antitumor agents, were prepared Thus, reaction of 2-amino-5-chlorothiazole.HCl with 2-quinolinethiol in the presence of NaHCO3 in DMF at 110° afforded I [R1 = 2-NH2; AR2 = 5-(2-quinolylthio)-; X = CH] which showed 74% increase in platelet number at 100 mg/kg in male ddY mice.

IT **183548-92-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiazoles and thiadiazoles for treatment of thrombocytopenia)
RN 183548-92-7 HCAPLUS
CN 2-Thiazolamine, 5-(4-quinazolinylsulfinyl)- (9CI) (CA INDEX NAME)

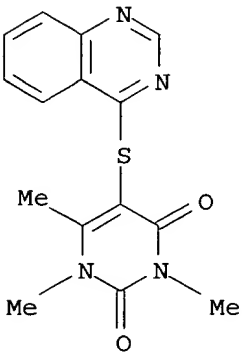


L13 ANSWER 22 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:731257 HCAPLUS
DOCUMENT NUMBER: 123:339501
TITLE: Reactions of diazines with nucleophiles. IV. The reactivity of 5-bromo-1,3,6-trimethyluracil with thiolate ions - substitution versus X-philic versus single electron transfer reactions
AUTHOR(S): Kumar, Subodh; Chimni, Swapandeep Singh; Cannoo, Deepika; Arora, Jasbir Singh
CORPORATE SOURCE: Department Chemistry, Guru Nanak Dev University, Amritsar, 143 005, India
SOURCE: Bioorganic & Medicinal Chemistry (1995), 3(7), 891-7
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reaction of 5-bromo-1,3,6-trimethyluracil with alkylthiolate (propane-1-, toluene-α-, allyl-, etc.) ions under phase transfer catalytic conditions follows nucleophilic substitution and X-philic (Br and S) elimination to give 5-alkylthio-1,3,6-trimethyluracils, 6-alkylthiomethyl-1,3-dimethyluracils and 1,3,6 -trimethyluracil. Reaction of 5-bromo-1,3,6-trimethyluracil with heteroarylthiolate ions (pyridine-2-, quinazoline-4-, uracil-2- and 4,6-dimethylpyrimidine-2-thiolate) gives only nucleophilic substitution products. However, arylthiolate (phenyl-, 4-chlorophenyl-, 2-aminophenyl-) ions follow a single electron transfer (SET) mechanism to give 5-arylthio-6-arylthiomethyl-1,3-dimethyluracils along with normal substitution products. 1,3,6-Trimethyluracil does not react with alkyl- or heteroaryl-thiolate ions but reacts with arylthiolate ions (SET) providing mainly 5-arylthio-1,3,6-trimethyluracils.
IT **170504-08-2P 170504-11-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactions of 5-bromo-1,3,6-trimethyluracil with thiolate ions)
RN 170504-08-2 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl-5-(4-quinazolinylthio)-6-[(4-quinazolinylthio)methyl]- (9CI) (CA INDEX NAME)



RN 170504-11-7 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1,3,6-trimethyl-5-(4-quinazolinylthio)- (9CI) (CA INDEX NAME)



L13 ANSWER 23 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:70632 HCAPLUS
DOCUMENT NUMBER: 108:70632
TITLE: Use of heterocyclic nitrogen-containing compounds for reducing moisture loss from plants and increasing crop yield
INVENTOR(S): Manning, David Treadway; Cappy, James Joseph; Cooke, Anson Richard; Sheads, Richard Eric; Wu, Tai Teh; Lopes, Anihal; Phillips, Jennifer Lyn; Outcalt, Russell James
PATENT ASSIGNEE(S): Union Carbide Agricultural Products Co., Inc., USA
SOURCE: PCT Int. Appl., 789 pp.
CODEN: PIXXD2

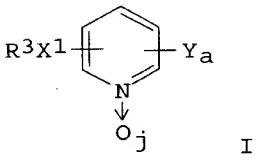
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8704321	A2	19870730	WO 1987-US240	19870123
WO 8704321	A3	19871105		
W: AU, BR, DK, FI, HU, JP, KR, LK, MW, NO, RO, SD, SU				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DD 254318	A5	19880224	DD 1987-299404	19870122
ZA 8700480	A	19880928	ZA 1987-480	19870122
ES 2004071	A6	19881201	ES 1987-158	19870122
AU 8770316	A1	19870814	AU 1987-70316	19870123
EP 258391	A1	19880309	EP 1987-901826	19870123
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
BR 8705356	A	19880405	BR 1987-5356	19870123
JP 63502511	T2	19880922	JP 1987-501343	19870123
HU 45848	A2	19880928	HU 1987-1236	19870123
FI 8704111	A	19870921	FI 1987-4111	19870921
DK 8704961	A	19870922	DK 1987-4961	19870922

PRIORITY APPLN. INFO.:

US 1986-824389	A	19860123
US 1986-939416	A	19861215
WO 1987-US240	A	19870123

GI

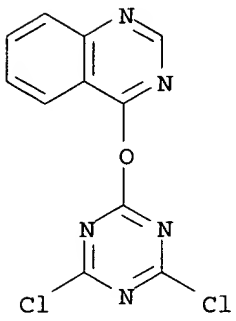


I

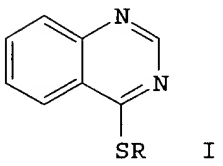
AB The title compds. R1XR2 [R1 = (un)substituted carbocyclic (aromatic or nonarom.) or heterocyclic ring; X = covalent single or double bond, (un)substituted heteroatom or substituted C, etc.; R2 = (un)substituted heterocyclic ring] are plant antitranspirants. The pyridines I [R3 = (un)substituted Ph, 1- or 2-naphthyl or heteroaryl; X1 = O, S, SO2, NH, CH2O, CH2S, etc.; Y = halo, alkyl, CN, polyhaloalkyl, alkoxy, etc.; a = 2-4, j = 0, 1] are novel compds. A solution of 12.4 g 4-methylthiophenol and 10.7 g 2,6-lutidine in 50 mL acetone was treated with 18.4 g cyanuric chloride in 200 mL acetone, to give 1.16 g 2,4-dichloro-6-(4-methylphenylthio)-1,3,5-triazine (II). II (1840 ppm) very markedly decreased transpiration rate and increased leaf diffusion resistance, in potted bean (Phaseolus vulgaris). In isolated pea chloroplasts, 2,4-dichloro-6-(2,6-dichlorophenoxy)-1,3,5-triazine (622 g/L) had no effect on photosynthetic electron transport, as shown by absence of O uptake inhibition. This was contrasted to 65% O uptake inhibition caused by the standard atrazine (108 g/L).

IT **112720-19-1P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as plant antitranspirant)
RN 112720-19-1 HCAPLUS
CN Quinazoline, 4-[(4,6-dichloro-1,3,5-triazin-2-yl)oxy]- (9CI) (CA INDEX NAME)



L13 ANSWER 24 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1986:199594 HCAPLUS
DOCUMENT NUMBER: 104:199594
TITLE: The synthesis and biological properties of the derivatives of 4-heterylmercaptoquinazoline
AUTHOR(S): Sinyak, R. S.; Mazur, I. A.; Stets, V. R.; Martynovskii, A. A.; Steblyuk, P. N.
CORPORATE SOURCE: Zaporozh. Med. Inst., Zaporozhe, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1986), 20(2), 168-71
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 104:199594
GI



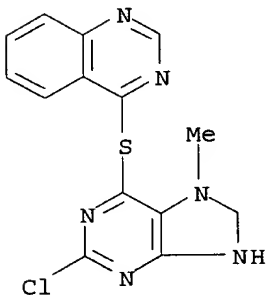
I

AB Nine title compds. (I; R = quinolyl, nitroquinolyl, chloromethylpurinyl, or substituted acridinyl) were prepared by reaction of 4-chloroquinazoline [5190-68-1] with 2-mercaptoquinoline [2637-37-8] or with mercaptoacridines, or by reaction of 4-mercaptoquinazoline [3337-86-8] with 4-methoxy-9-chloroacridine [16492-15-2], 5-nitro-8-chloroquinoline [22539-55-5], or 2,6-dichloro-7-methylpurine [2273-93-0]. Analgesic activity in mice was exhibited in I with a 5-nitroguinolin substituent or with an acridine ring substituted in the 2-postion. Substitution with 5-nitroquinoline also reduced I toxicity. Various I exhibited anti-inflammatory and sleep-prolonging activity in mice, and some I displayed antimicrobial activity in vitro. Various structure-activity relations of I are discussed.
IT **102244-05-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. activity of, structure in relation to)

RN 102244-05-3 HCAPLUS

CN 1H-Purine, 2-chloro-7,8-dihydro-7-methyl-6-(4-quinazolinylthio)- (9CI) (CA INDEX NAME)



L13 ANSWER 25 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1984:603875 HCAPLUS

DOCUMENT NUMBER: 101:203875

TITLE: Nitroimidazoles: part XIX - structure-activity relationships

AUTHOR(S): Nagarajan, K.; Arya, V. P.; George, T.; Nair, M. D.; Sudarsanam, V.; Ray, D. K.; Shrivastava, V. B.

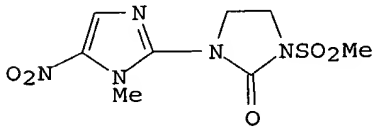
CORPORATE SOURCE: Res. Cent., CIBA-GEIGY, Bombay, 400 063, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(4), 342-62
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

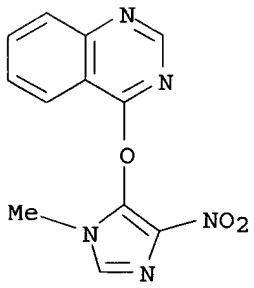
AB A variety of nitroimidazoles, mostly 1,2-disubstituted-5-nitro derivs. were examined for in vitro activity against Entamoeba histolytica and for effectiveness in treating early hepatic infection in golden hamsters. Many compds. carried a functionalized N atom at position 2. In vivo activity was observed with 1-alkyl-5-nitroimidazoles carrying a substituted imidazolidinone or imidazole. Among these derivs., 1-methylsulfonyl-3-(1-methyl-5-nitro-2-imidazolyl)-2-imidazolidinone (I) [56302-13-7] was the most potent against hepatic and caecal infections of E. histolytica in the golden hamster and Trichomonas foetus infections in mice. It was developed as a drug for treatment of amoebiasis, giardiasis, and trichomoniasis. The structure-antiamebic activity relationships of the

nitroimidazoles are discussed.

IT **86231-03-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(amebicidal activity of, structure in relation to)

RN 86231-03-0 HCAPLUS

CN Quinazoline, 4-[(1-methyl-4-nitro-1H-imidazol-5-yl)oxy]- (9CI) (CA INDEX NAME)



L13 ANSWER 26 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:422379 HCAPLUS

DOCUMENT NUMBER: 99:22379

TITLE: Nitroimidazoles. Part XVI. Some 1-methyl-4-nitro-5-substituted imidazoles

AUTHOR(S): Arya, V. P.; Nagarajan, K.; Shenoy, S. J.

CORPORATE SOURCE: Ciba-Geigy Res. Cent., Bombay, 400 063, India

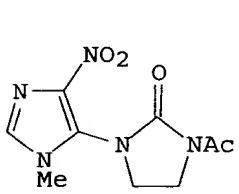
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1982), 21B(12), 1115-17
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

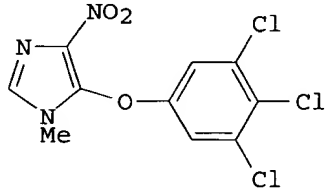
LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:22379

GI



II

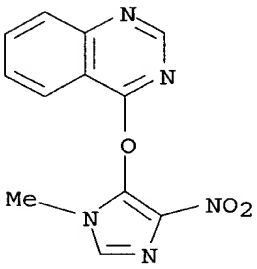


III

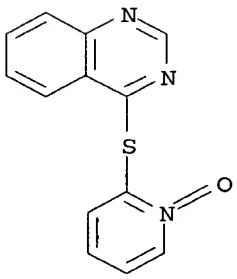
AB Treatment of 1-methyl-4-nitro-5-chloroimidazole I with 5-membered lactams, e.g. imidazolidinones, oxazolidinone, and thiazolidinone, and imidazole affords N-imidazolyl derivs., e.g. II. Amino derivs. are similarly obtained. 2-Hydroxypyrazine, 4-hydroxyquinazoline, and 3,4,5-trichlorophenol and I react to form O-derivs., e.g. III, while mercaptans provide the sulfides.

IT **86231-03-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 86231-03-0 HCAPLUS
CN Quinazoline, 4-[(1-methyl-4-nitro-1H-imidazol-5-yl)oxy]- (9CI) (CA INDEX NAME)



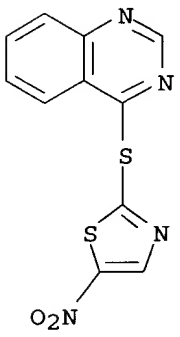
L13 ANSWER 27 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:582339 HCAPLUS
DOCUMENT NUMBER: 97:182339
TITLE: Quinazolines, their preparation and biological activity
AUTHOR(S): Schoenowsky, Hubert; Sachse, Burkhardt
CORPORATE SOURCE: Pflanzenschutzforsch.-Chem., Hoechst A.-G., Frankfurt/Main, D-6230/80, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1982), 37B(7), 907-11
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: German
AB 4-Hydroxyquinazolines (I) were prepared by cyclocondensation of 2-aminobenzoic acids with formamide and were alkylated and arylated to give alkoxy- and (aryloxy)quinazolines. 4-Chloroquinazolines were prepared by treatment of I with PCl5/POCl3 and were converted into thio and amino compds. by reaction with mercaptans and amines, resp. A number of the quinazolines showed fungicidal activity.
IT **83529-97-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 83529-97-9 HCAPLUS
CN Quinazoline, 4-[(1-oxido-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)



L13 ANSWER 28 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:4286 HCAPLUS
DOCUMENT NUMBER: 78:4286
TITLE: 5-Nitro-2-thiazolyl sulfides
INVENTOR(S): Hughes, Peter Graham; Verge, John Pomfret
PATENT ASSIGNEE(S): Lilly Industries Ltd.
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2213558	A	19721005	DE 1972-2213558	19720321
GB 1354296	A	19740522	GB 1971-8252	19710330
US 3870725	A	19750311	US 1972-234376	19720313
CH 545812	A	19740215	CH 1972-4021	19720316
IT 965768	A	19740211	IT 1972-49259	19720327
FR 2132133	A5	19721117	FR 1972-10848	19720328
FR 2132133	B1	19750620		
PRIORITY APPLN. INFO.:			GB 1971-8252 A	19710330
			GB 1971-39106 A	19710820

GI For diagram(s), see printed CA Issue.
AB Forty-five title compds. (I, R = substituted 1.3,4-thiadiazol-k-yl, 5-thioxo-1.3,4-chiadiazol-2-yl, 1.3,4-oxadiazol-k-yl, 1.2,4-triazol-1(or 5)-yl, 1.2,3,4-tetrazol-5-yl, 1.2,4-triazin-1-yl, 4-quinazolinyl, 2-pyrimidinyl, 2(or 4)-pyridyl, or 2-quinolyl), useful as fungicides, were prepared by reaction of the bromo derivative II with RSX (X = H, K, Na).
IT **40045-66-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40045-66-7 HCAPLUS
CN Quinazoline, 4-[(5-nitro-2-thiazolyl)thio]- (9CI) (CA INDEX NAME)



L13 ANSWER 29 OF 29 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:413319 HCAPLUS
DOCUMENT NUMBER: 71:13319
TITLE: Glycosides and heterocycles. XXXV. Glycosides of hydroxy- and mercaptoquinazolines
AUTHOR(S): Wagner, Guenther; Suess, F.

CORPORATE SOURCE: Pharm, Inst., Karl-Marx-Univ., Leipzig, Fed. Rep. Ger.
SOURCE: Pharmazie (1969), 24(1), 35-8
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German

GI For diagram(s), see printed CA Issue.

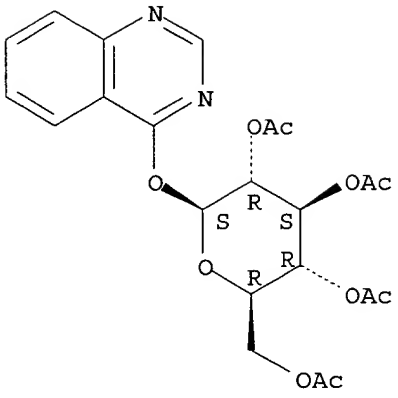
AB 4-Hydroxyquinazoline (I) Ag salt (7.59 g.) was mixed with 300 ml. C6H6, 250 ml. solvent was distilled, a solution of 4.11 g. tetra-O-acetyl-α-D-glucopyranosyl bromide (II) added, the mixture refluxed 2 hrs. and filtered, the filtrate evaporated, and the residue purified by thin-layer chromatog. on SiO2 in the solvent system 3:2 AcOEt-cyclohexane to yield 40% 4-(tetra-O-acetyl-β-D-glucopyranosyloxy)quinazoline (III) (Q = tetra-O-acetyl-β-D-glucopyranosyl throughout this abstract), m. 150-2° (MeOH), [α]20D -22.5° (c 2.5, CHCl3). I Hg salt (1.62 g.) and 2.71 g. II refluxed for 2 hrs. in 100 ml. MePh and filtered, the filtrate washed with Na2S2O3 and 5% NaOH and evaporated gave, after addition of MeOH, 50% 3-(tetra-O-acetyl-β-D-glucopyranoysl)-4-quinazolinone (IVa), m. 192-4° (70% MeOH), [α]20D 0° (CHCl3). III (0.52 g.) and 2.02 g. HgBr2 refluxed 2 hrs. in 50 ml. anhydrous PhMe afforded 80% IVa. IVa deacetylated by heating in 0.05M MeONa gave 70% 3-β-D-glucopyranosyl-4-quinazolinone (IVb) (G = β-D-glucopyranosyl throughout this abstract), m. 257.5-8.5° (PrOH), [α]20D 37.3° (c 2.3, HCONMe2). A solution of 1.82 g. 2,3,4,6-tetra-O-acetyl-1-thio-β-D-glucopyranose and 0.82 g. 4-chloroquinazoline in 16 ml. Me2CO was treated with 0.28 g. KOH in 4 ml. H2O, agitated 25 min., and diluted with 100 ml. H2O to yield 84% 4-(tetra-O-acetyl-β-D-glucopyranosylthio)quinazoline (Va), m. 95-6° (MeOH), [α]20D 12° (c 3, CHCl3). 2-Chloroquinazoline gave similarly 40% 2-(tetra-O-acetyl-β-D-glucopyranosylthio)quinazoline (VIa), m. 143-5° (30% MeOH), [α]20D 13° (c 3, CHCl3). A mixture of 0.5 g. IVa and 1.2 g. P4S10 in 5 ml. anhydrous C5H5N heated 5 hrs. at 130° and 10 hrs. at 160°, cooled, extracted repeatedly with CHCl3, the combined exts. washed with 5% NaOH, evaporated, and the residue treated with MeOH, gave 70% 3-(tetra-O-acetyl-β-D-glucopyranosyl)-4-quinazolinethione (VII), m. 174.5-5.5° (50% MeOH), [α]20D 7° (c 2.2, CHCl3). The reaction of 4-quinazolinethiol and II in aqueous Me2CO in the presence of NaOH yielded 56% Va and 8% VII. Deacetylation of Va with MeOH gave 85% 3-β-D-glucopyranosyl-4-quinazolinethione (Vb), m. 218-20° (PrOH), [α]20D -19° (c 3.4, HCONMe2). The reaction of 2-hydroxyquinazoline and II in aqueous Me2CO in the presence of NaOH followed by preparative thin-layer chromatog. on SiO2 in 3:2 C6H6-EtOAc gave 5% 2-(tetra-O-acetyl-β-D-glucopyranosyloxy)quinazoline, m. 119-21° (35% MeOH), [α]20D 8° (c 2.5, CHCl3). 2-Quinazolinethiol reacted with II in aqueous Me2CO afforded 38% VIa. Deacetylation of VIa with MeONa gave 60% 2-(β-D-glucopyranosylthio)quinazoline (VIb), m. 113-15° (PrOH), [α]20D. -96.4° (c 2, HCONMe2). Uv spectrum of IVa was very similar to that of 3-methyl-4-quinazoline and differed from the spectrum of 1-methyl-4-quinazoline. This confirmed the structure of IVa.

IT **24558-70-1P 24577-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24558-70-1 HCAPLUS

CN Quinazoline, 4-(β-D-glucopyranosyloxy)-, 2',3',4',6'-tetraacetate (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 24577-13-7 HCAPLUS
CN Quinazoline, 4-(β-D-glucopyranosylthio)-, 2',3',4',6'-tetraacetate (8CI) (CA INDEX NAME)

Absolute stereochemistry.